Resolving Spontaneous Nonlinear Multi-Physics Flow Localisation in 3-D: Tackling Hardware Limit

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S9368 | 20 March 2019 | Nvidia GTC | Silicon Valley

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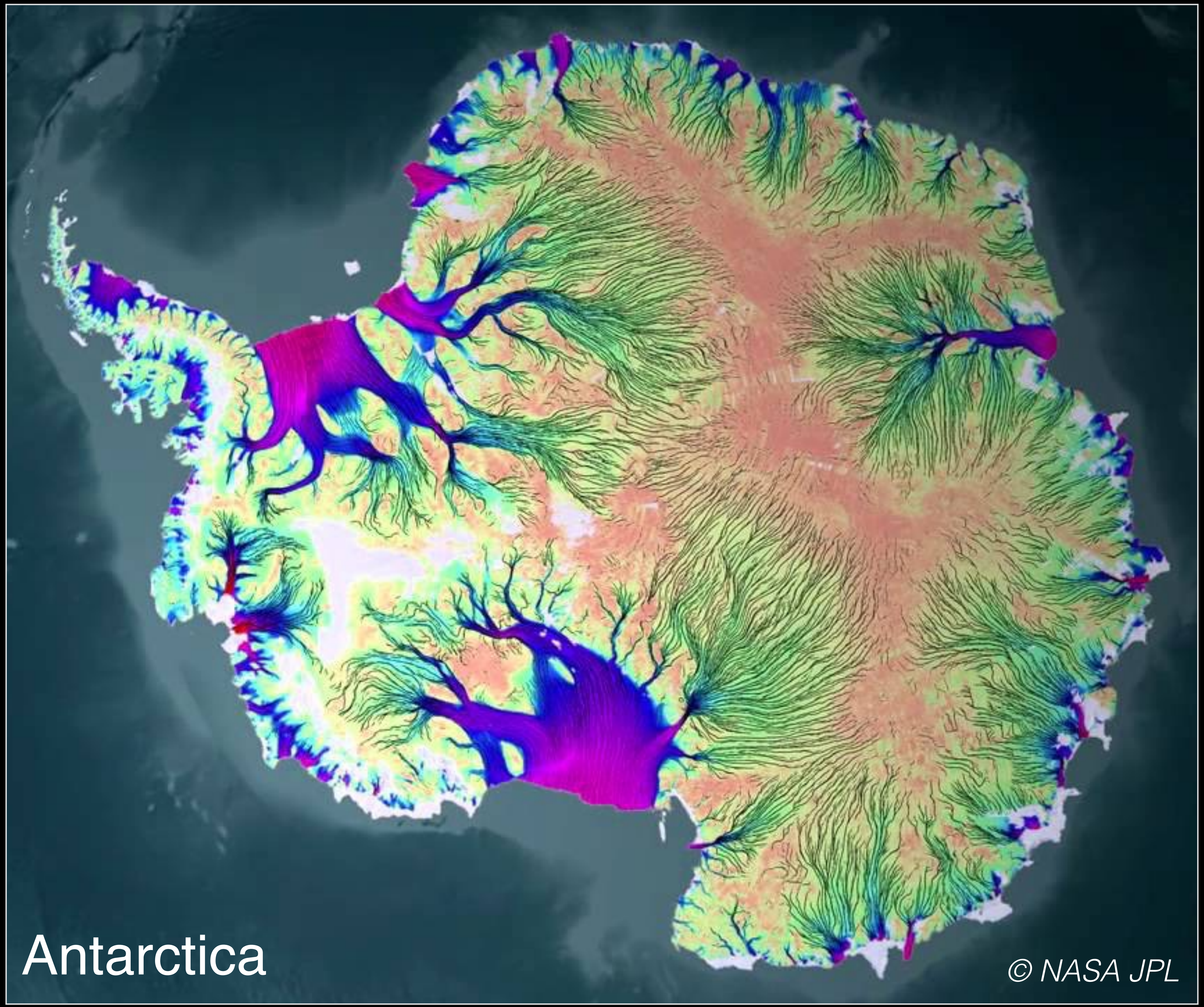
Multi-physics flow localisation




Subsurface reservoirs
Extraction and storage


Subsurface reservoirs
Extraction and storage
Pockmark
INT
H50
Truncations
H60
H70
Chimney
Løseth et al., 2011
Plaza-Faverola et al., 2011
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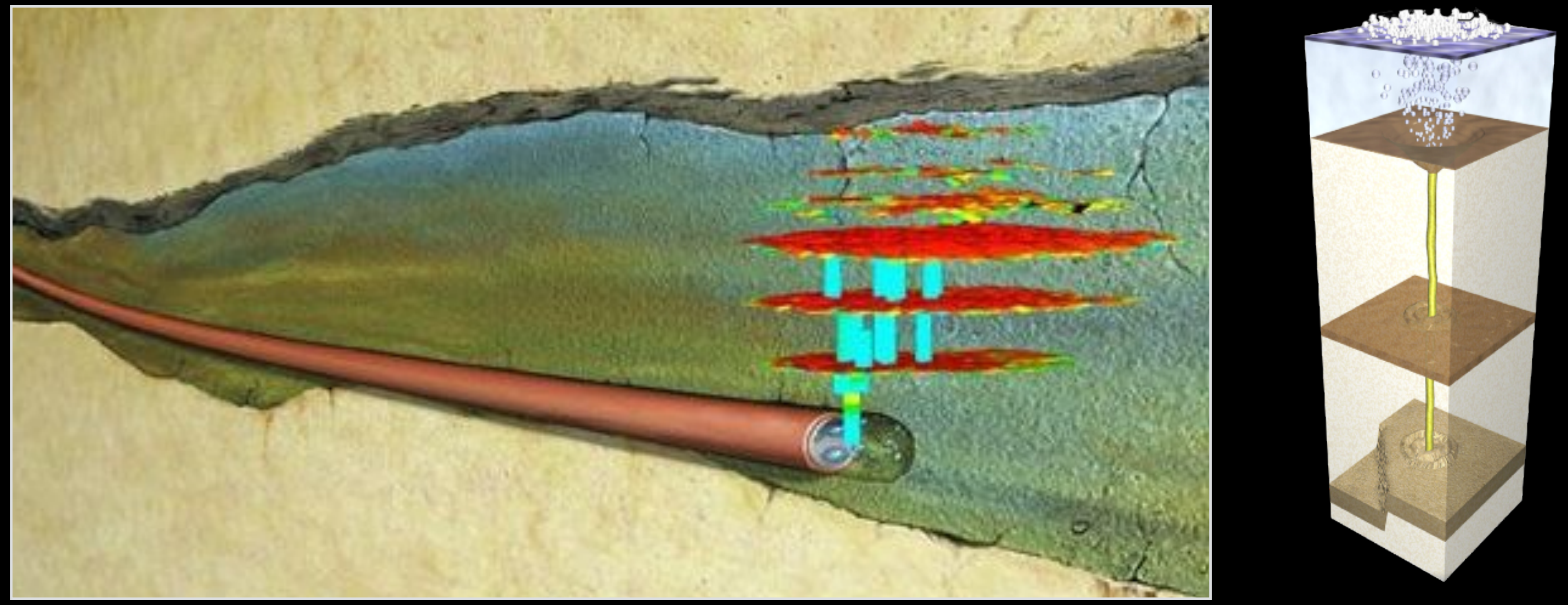
Why do we care

Fast flowing ice streams

> Impact sea-level rise



High-permeability chimneys

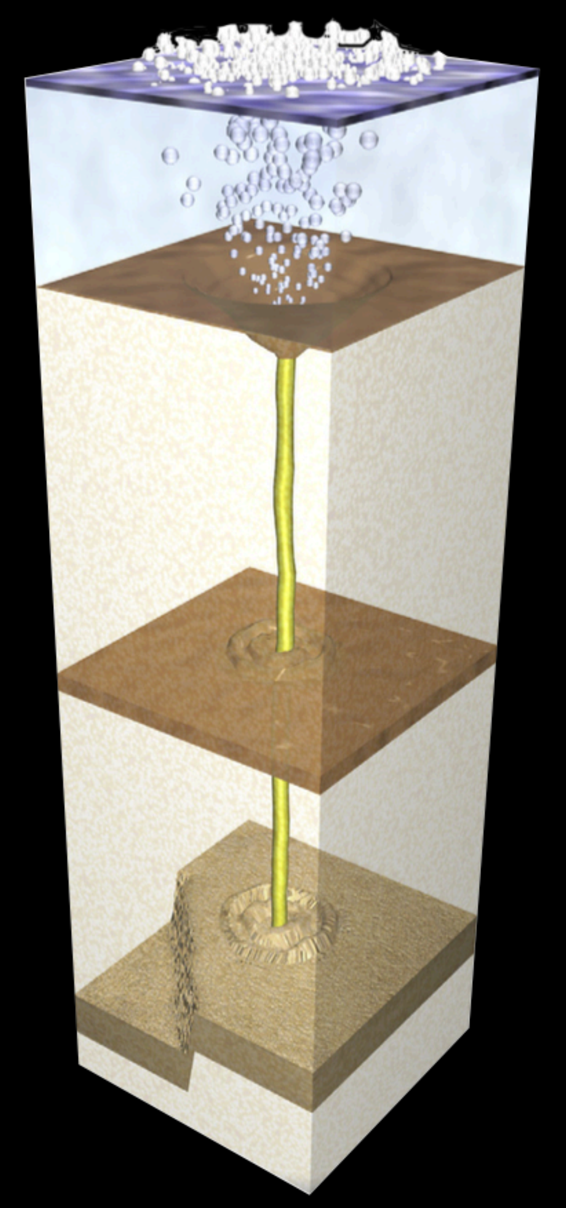
> Compromise safe CO_2 storage

- Macro-scale “reservoirs” | Micro-scale processes
- Multi-physics flow localisation trigger meso-scale instabilities
- Resolve the key physical processes to make accurate predictions

The challenge

Resolve meso-scale dynamics

- Develop predictive models to resolve nonlinear multi-physics processes
- Capture spontaneous localisation in space + time
- Large domains but highly localised action
- Computationally challenging:



The challenge

Resolve meso-scale dynamics

- Develop predictive models to resolve nonlinear multi-physics processes
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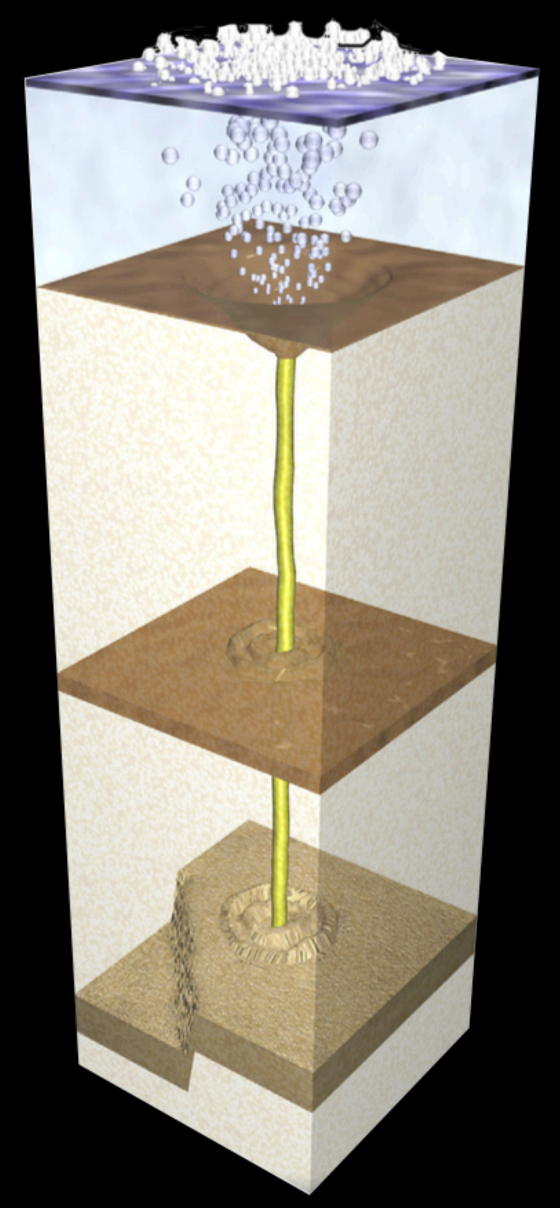
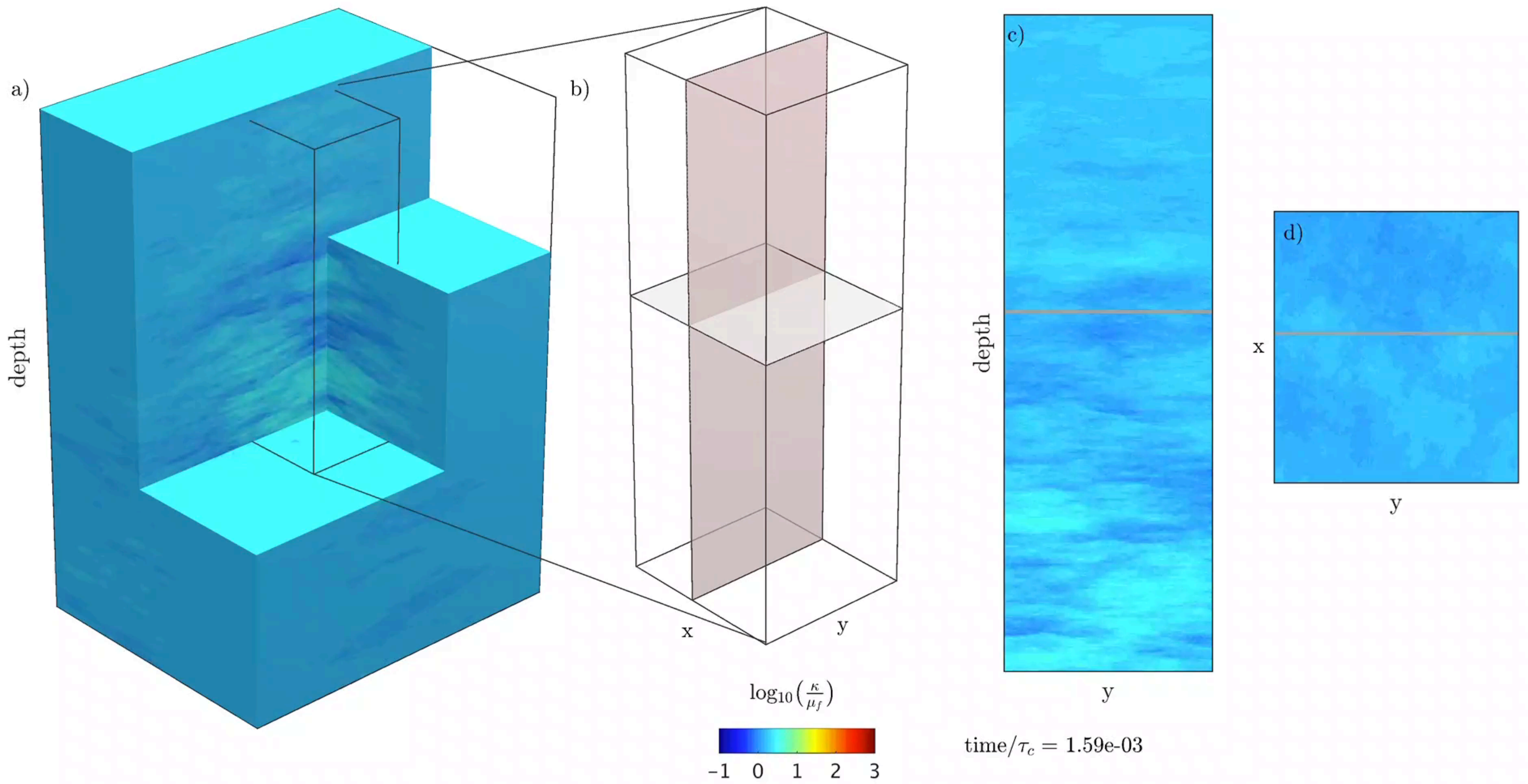
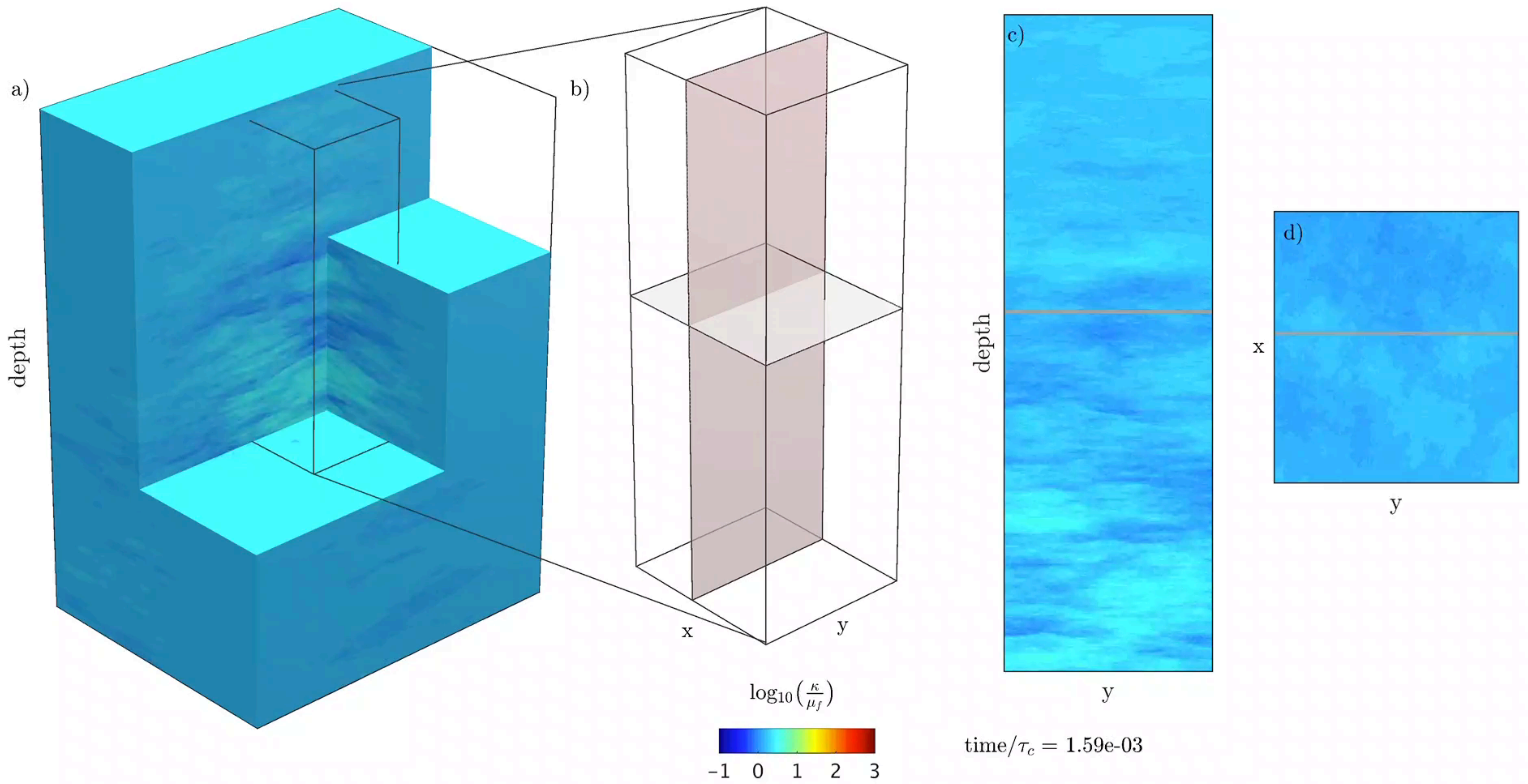
Extremely high-resolution 3-D forward models are mandatory

Requires a supercomputing approach





Räss et al., 2018. Nature Scientific Reports



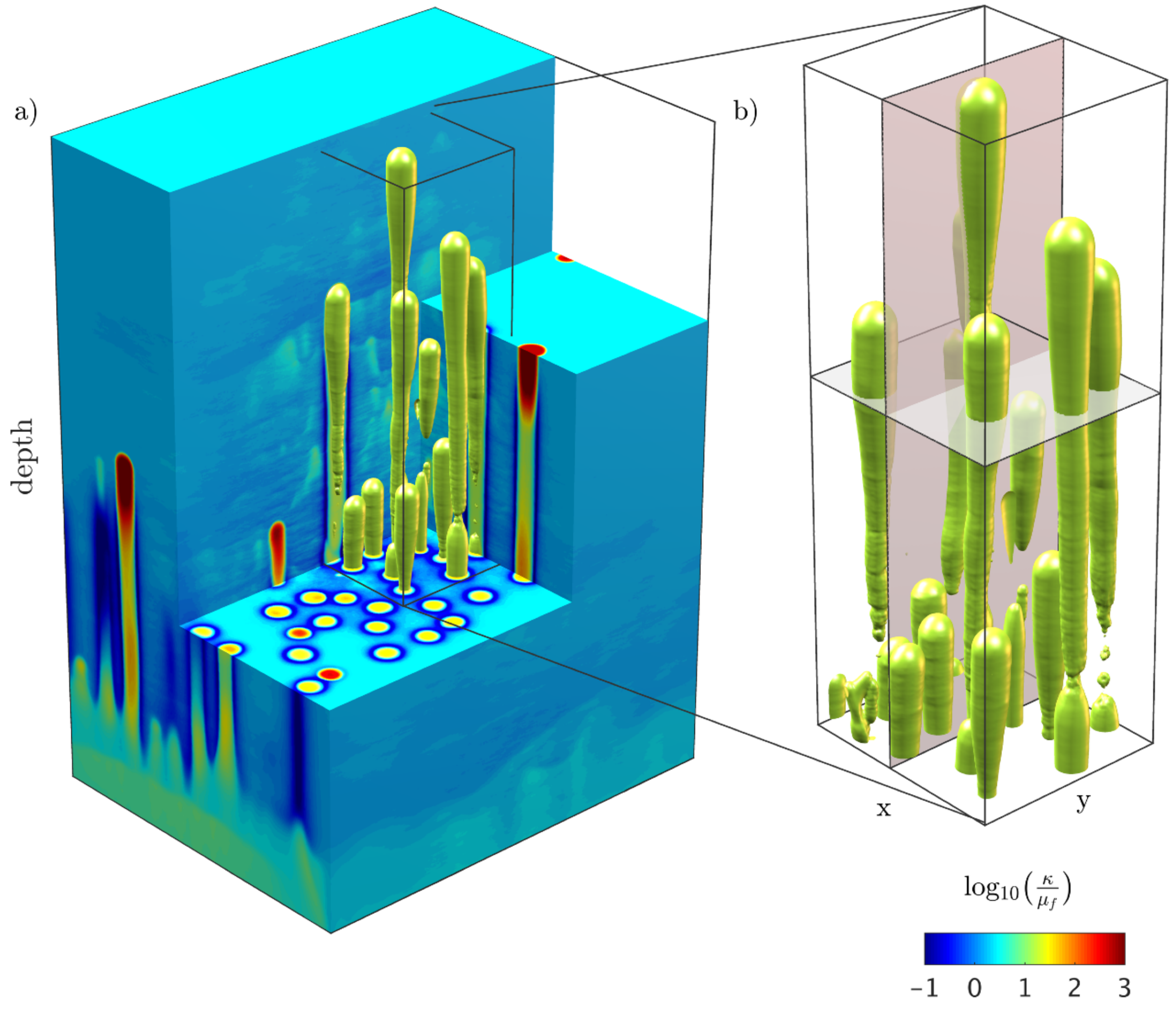
Räss et al., 2018. Nature Scientific Reports

Supercomputing in Earth Sciences

Resolution:

- space: 1000 x 1000 x 2000 grid points in 3-D
- time: 20’000 implicit time steps

- Finite-Difference method + staggered grid
- CUDA C + MPI
- 128 Titan Xm GPUs [home built supercomputer]
- ~600 GB memory footprint | 20 TB / 100 disk saves



Räss et al., 2018. Nature Scientific Reports

Supercomputing in Earth Sciences

SCIENTIFIC REPORTS

OPEN

Spontaneous formation of fluid escape pipes from subsurface reservoirs

Received: 29 March 2018

Ludovic Räss[1,2], Nina S. C. Simon[3] & Yury Y. Podladchikov[1,2]

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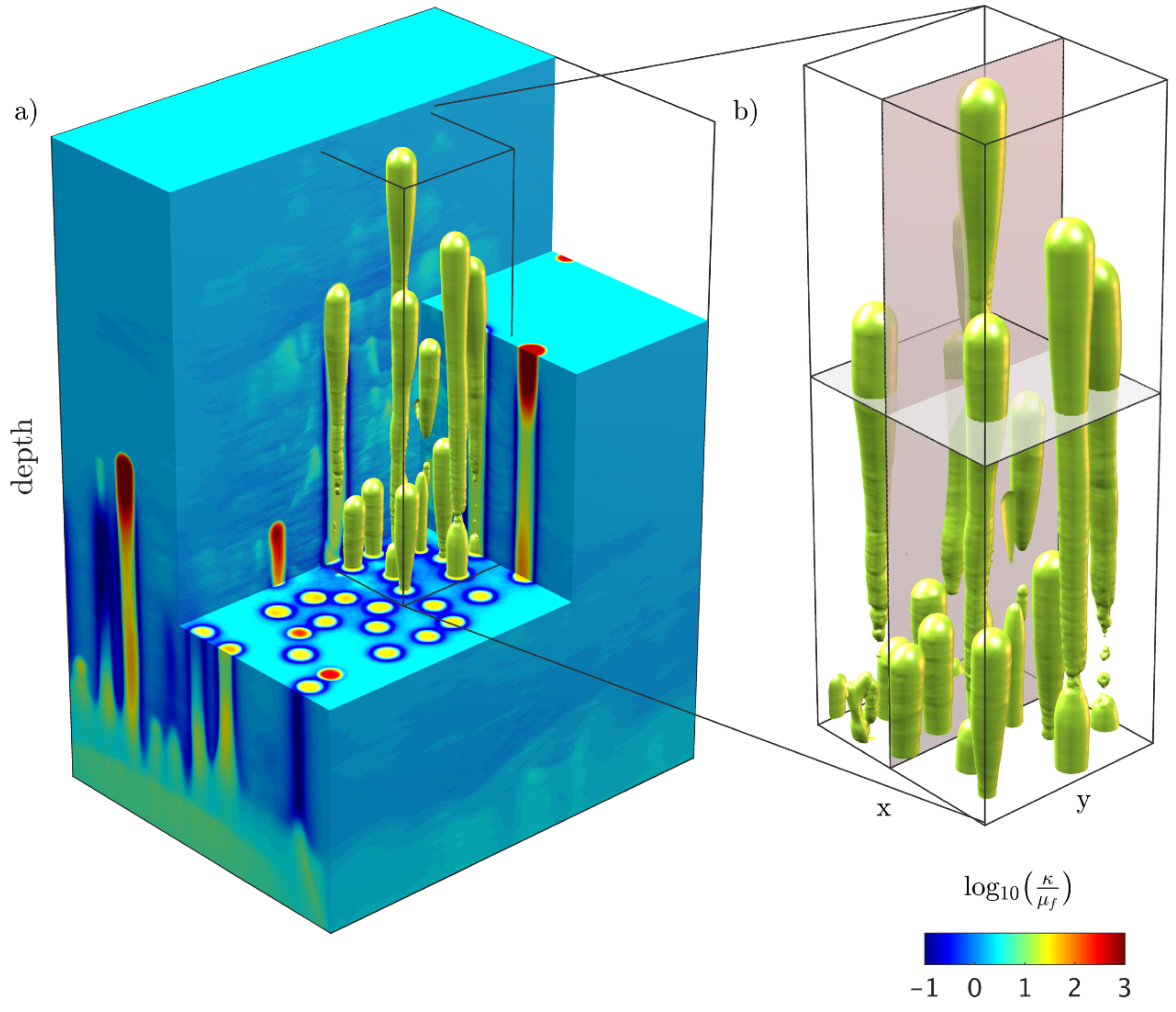
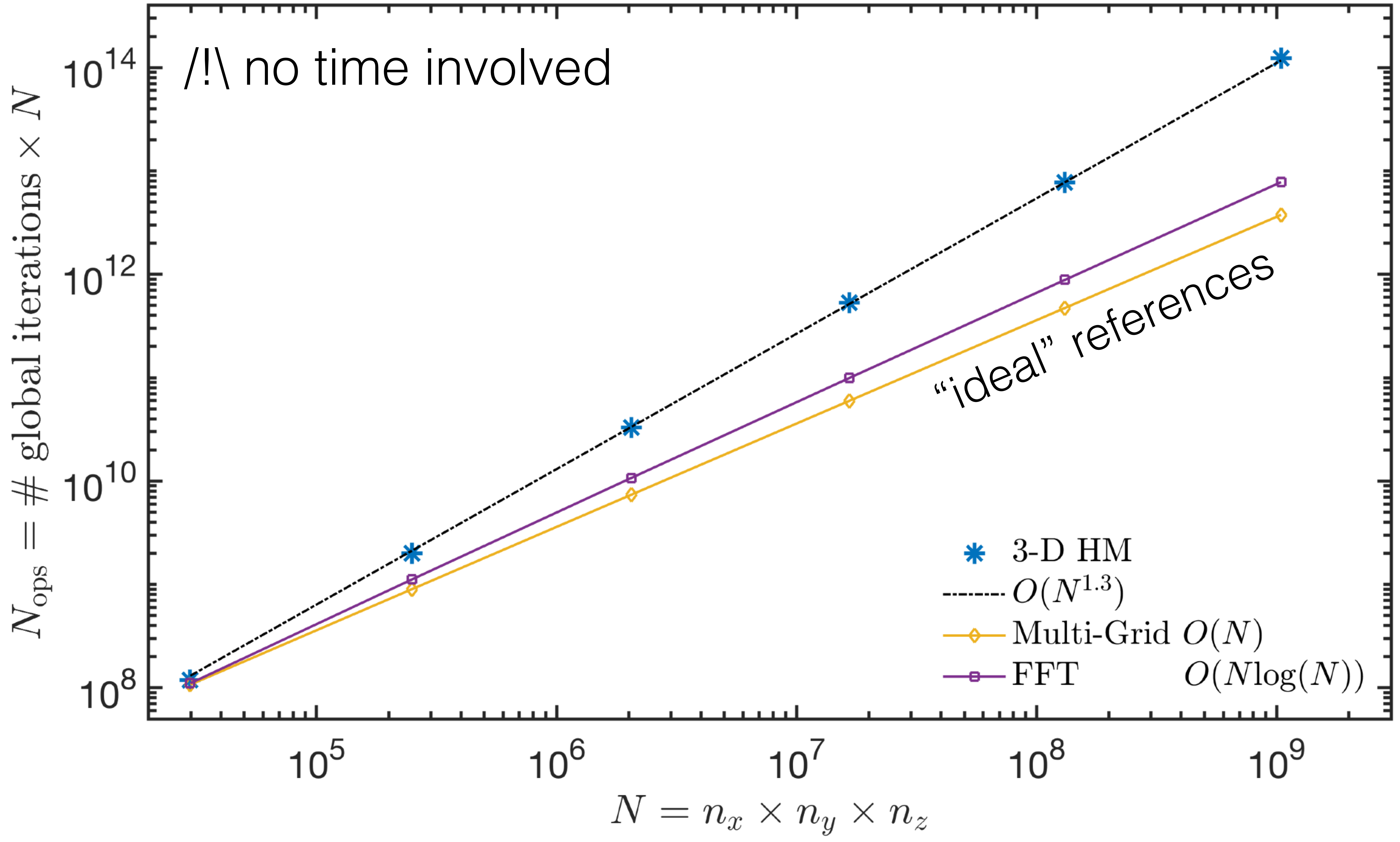


Runs close to hardware limit !

Räss et al., 2018. Nature Scientific Reports

1/ Pseudo-Transient solver

Scaling of our iterative GPU solver with numerical grid resolution N



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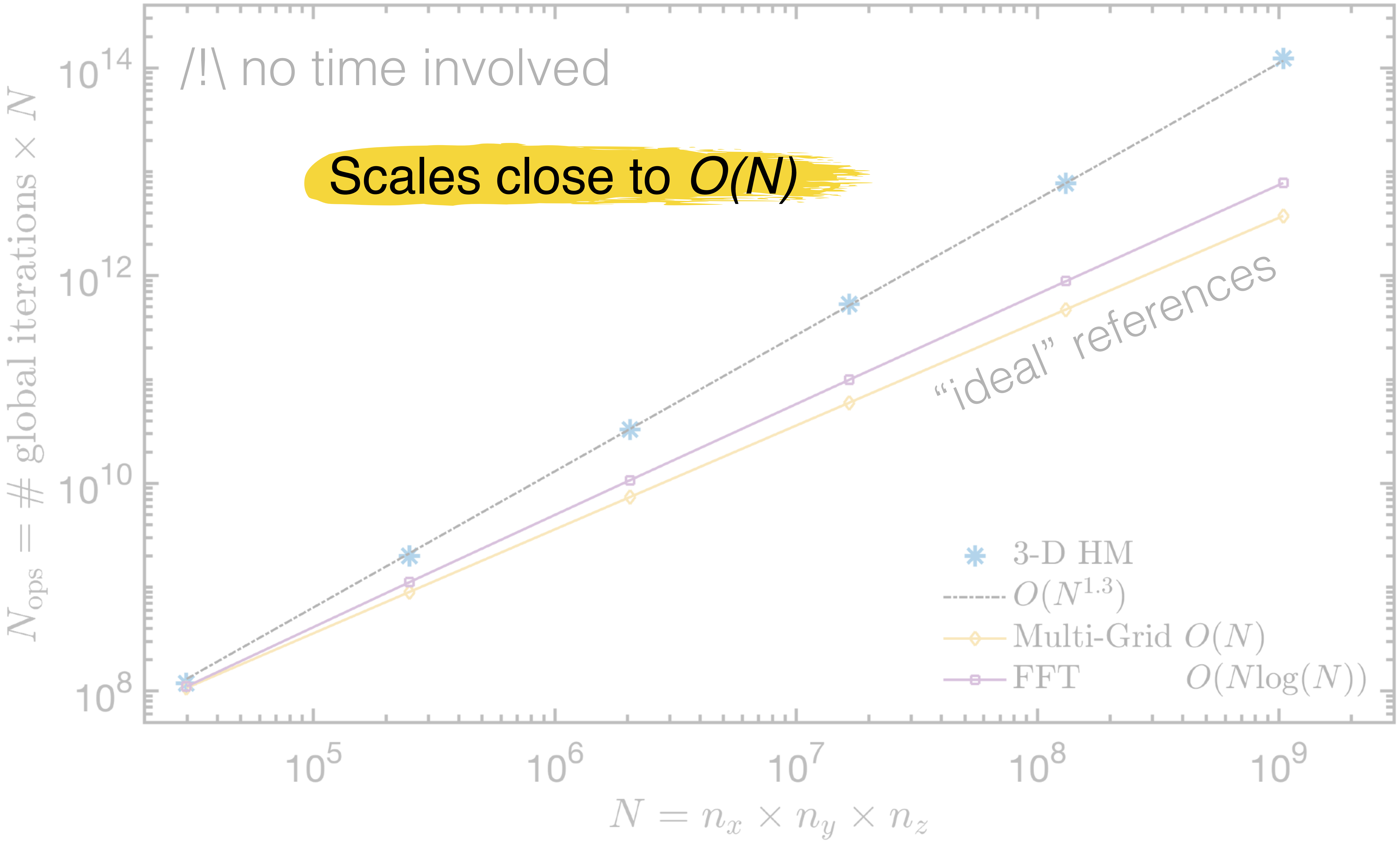
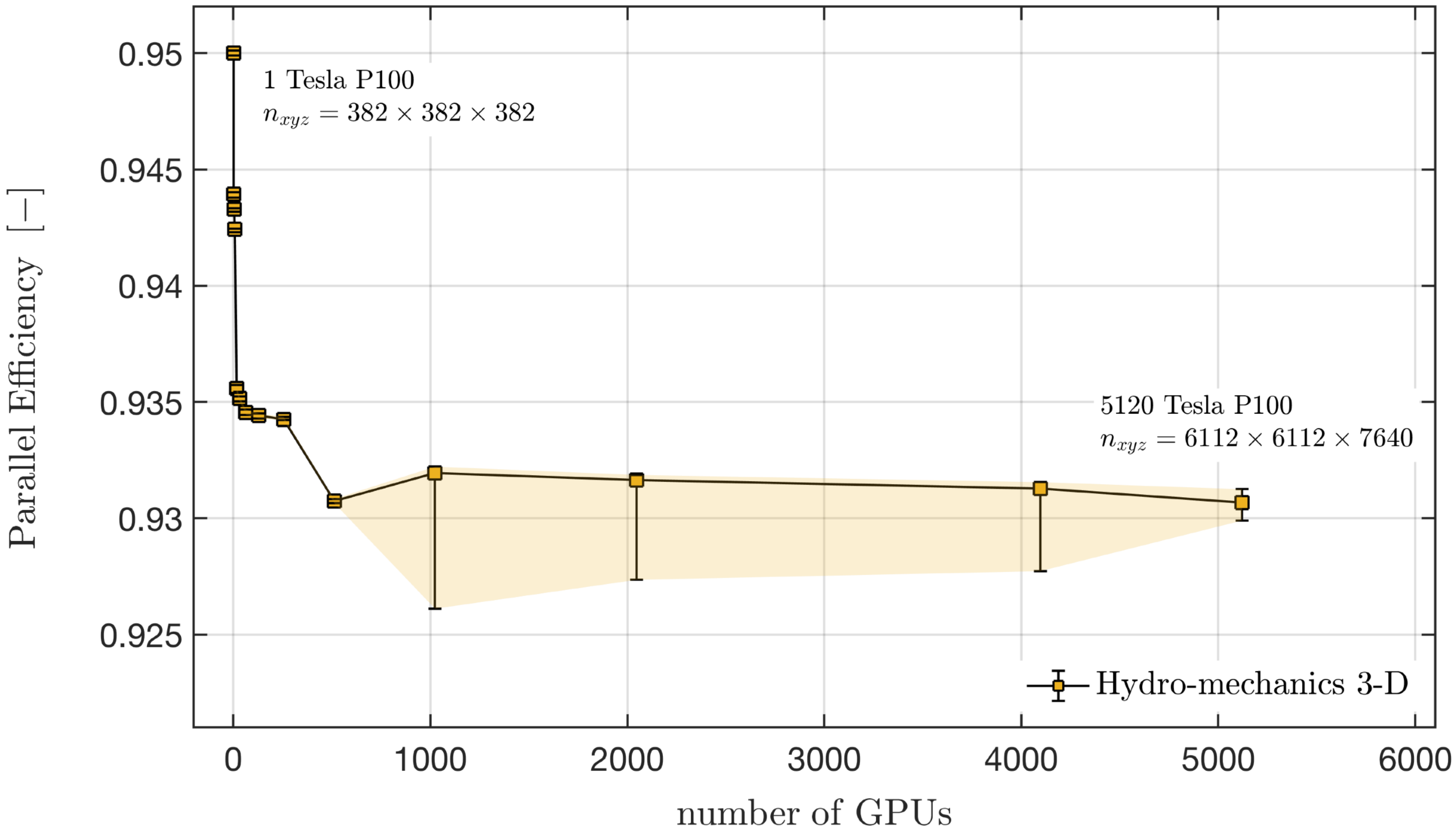
Scaling of our iterative GPU solver with numerical grid resolution N



2/ Hide MPI communication

Weak scaling on Cray XC50 “Piz Daint” @ CSCS | **5120 Nvidia P100 GPUs**



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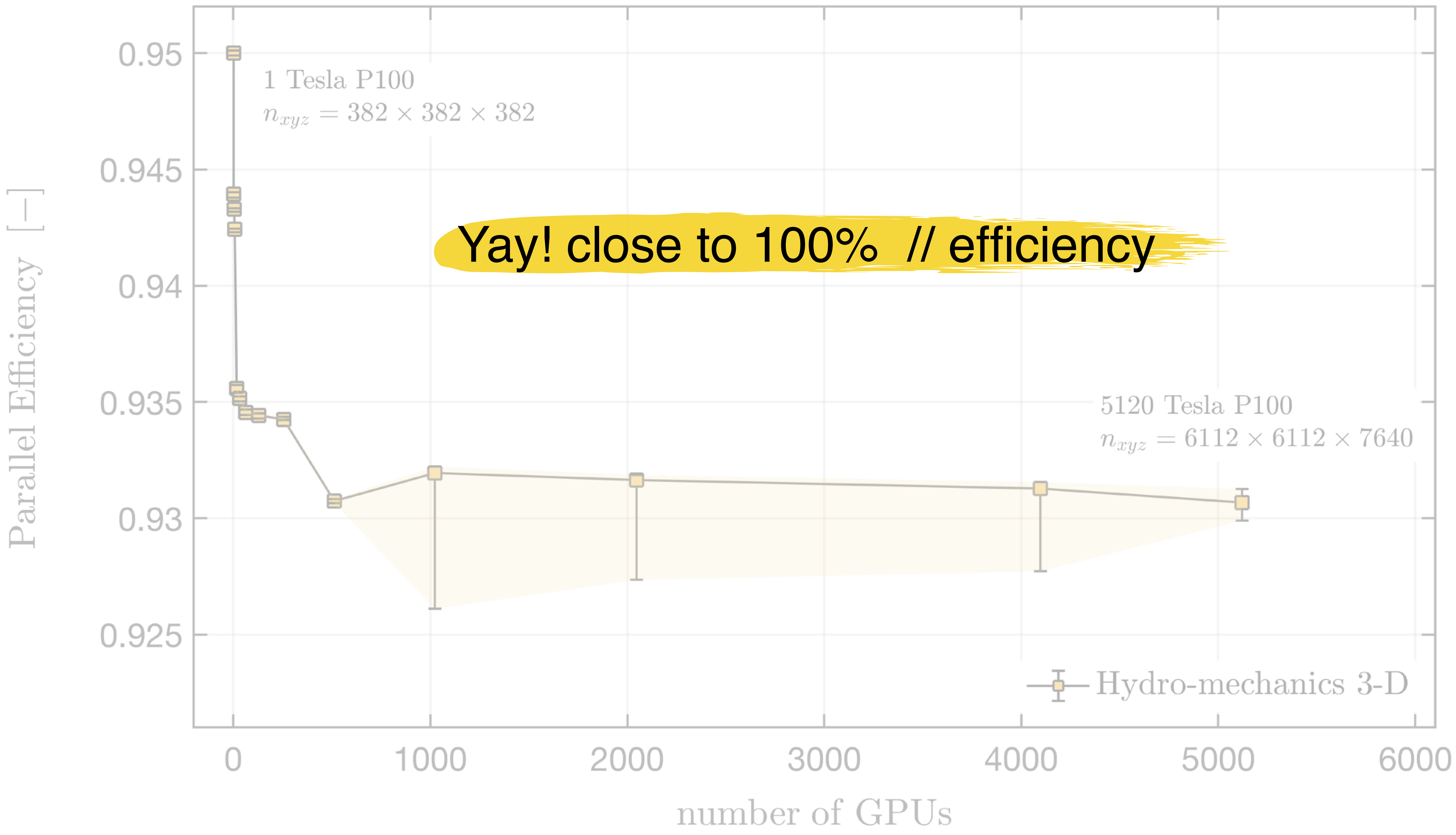

The road to a [fast] solution

Agenda

- Results ✓
- 1/ Pseudo-Transient - *be close to physics*
- 2/ Parallel efficiency - *hide MPI communication*
- Summary & Outlook
- Q&A

Solve 3-D solid / fluid mechanics

- Solve 3-D nonlinear hydro-mechanics PDEs | 15 mandatory fields to update

$$0 = \nabla_j(\bar{\tau}_{ij} - \bar{p}\delta_{ij}) - \bar{\rho}g_i$$

$$0 = \nabla_k v_k + \frac{\bar{p} - p^f}{\eta_\phi(1-\phi)}$$

$$0 = \nabla_k q_k^D - \frac{\bar{p} - p^f}{\eta_\phi(1-\phi)}$$

$$\frac{\partial \phi}{\partial t} = (1-\phi)\nabla_k v_k$$

$$\frac{\partial \bar{\tau}_{ij}}{\partial t} = f(v, G, \mu_s)$$

$$\eta_\phi = f(\phi, \bar{p}, p^f, \dot{\epsilon}_{II})$$

$$\mu = f(\phi, \dot{\epsilon}_{II})$$

$$k_\phi = k_0(\phi/\phi_0)^3$$

Utilise a fully local physics-based iterative method: **Pseudo-Transient**

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Utilise a fully local physics-based iterative method: **Pseudo-Transient**

- Avoid being “killed” by global communication & memory footprint
- Exploit the low level parallelism of GPUs + available supercomputing power

1/ Pseudo-Transient iterations

A general approach

- e.g. solution to an elliptic problem:

$$C = \frac{\partial^2 A}{\partial x^2}$$

$$0 = \frac{\partial^2 A}{\partial x^2} - C = f_{\mathrm{A}}$$

1/ Pseudo-Transient iterations

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- Naive iterations (1st order):

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$$A^{[k+1]} = A^{[k]} + \Delta\tau_\mathrm{A} f_\mathrm{A}^{[k]}$$

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(pseudo) time step

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$$\begin{aligned} f_{\mathrm{v}} &= \nabla_j(\bar{\tau}_{ij} - \bar{p}\delta_{ij}) - \bar{\rho} g_i \\ f_{\bar{\mathrm{p}}} &= \nabla_k v_k + \frac{\bar{p} - p^f}{\eta_\phi(1-\phi)} \\ f_{\mathrm{p^f}} &= \nabla_k q_k^D - \frac{\bar{p} - p^f}{\eta_\phi(1-\phi)} \end{aligned}$$

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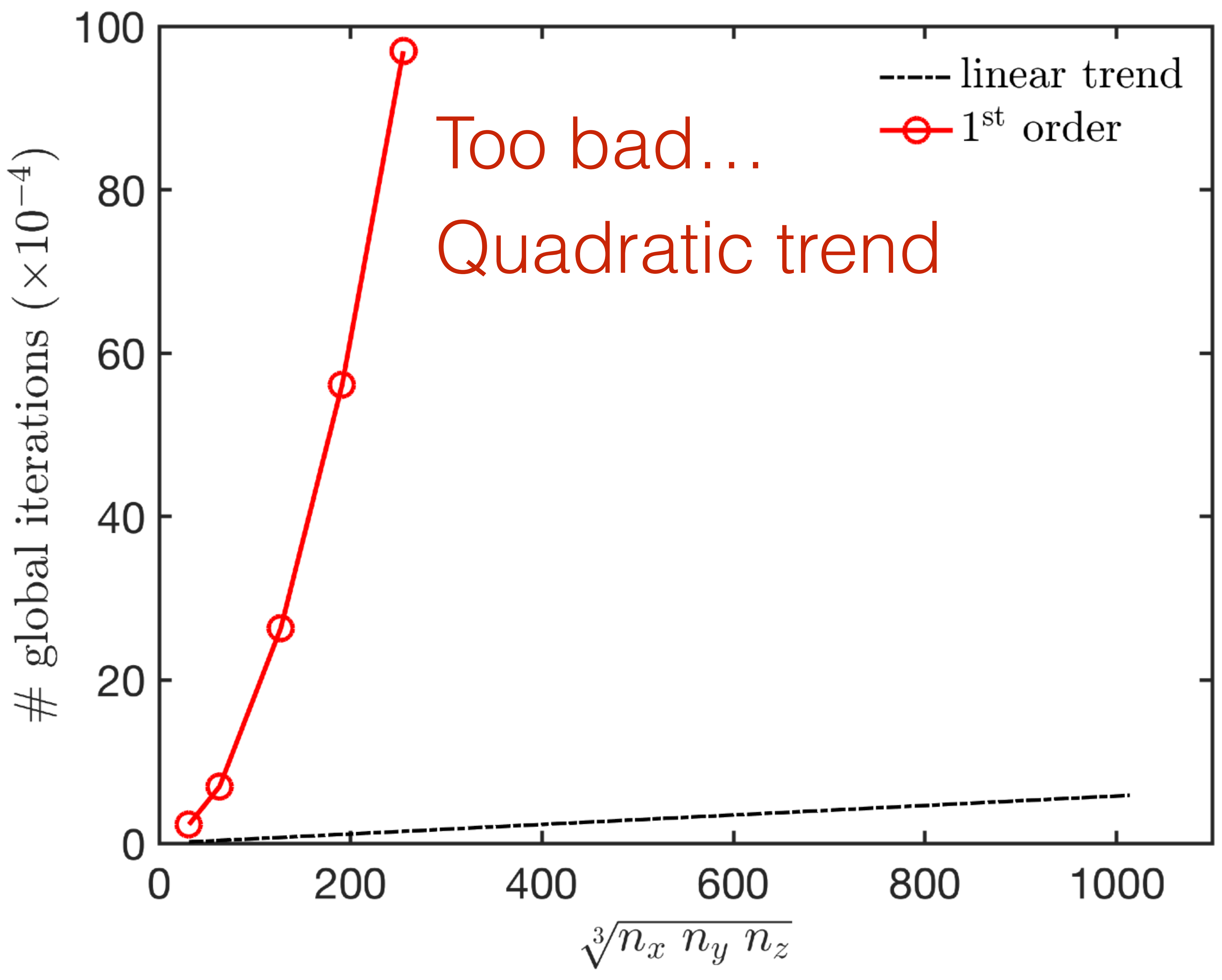
(pseudo) time step

Pseudo-Transient | naive

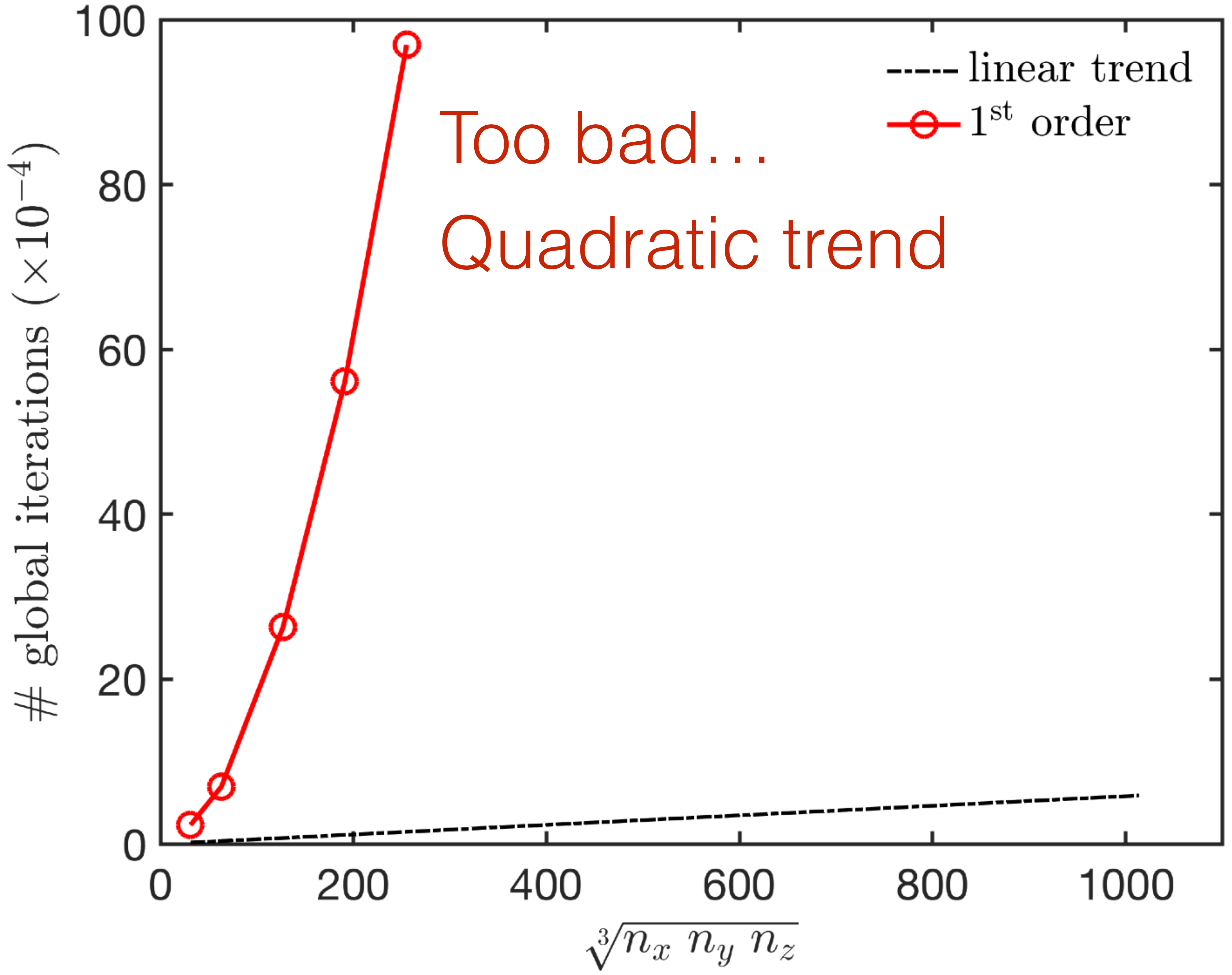
- 1st order scheme | 3-D hydro-mechanics



Pseudo-Transient | naive

- 1^{st} order scheme | 3-D hydro-mechanics

Simple - but does not scale with resolution increase



Pseudo-Transient iterations

An improved approach

- Second order iterations:

Frankel, 1950

$$\frac{\partial A}{\partial \tau_{\mathrm{A}}} = f_{\mathrm{A}}$$

$$A^{[k+1]} = A^{[k]} + \Delta\tau_{\mathrm{A}} \; f_{\mathrm{A}}^{[k]}$$

Pseudo-Transient iterations

An improved approach

- Second order iterations:

Frankel, 1950

$$\alpha \frac{\partial^2 A}{\partial \tau_A^2} + \frac{\partial A}{\partial \tau_A} = f_A$$

$$A^{[k+1]} = A^{[k]} + \Delta\tau_A \left(f_A^{[k]} + (1 - \nu/n_i)\, f_A^{[k-1]} \right)$$

Pseudo-Transient iterations

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damping

0 0 0 0

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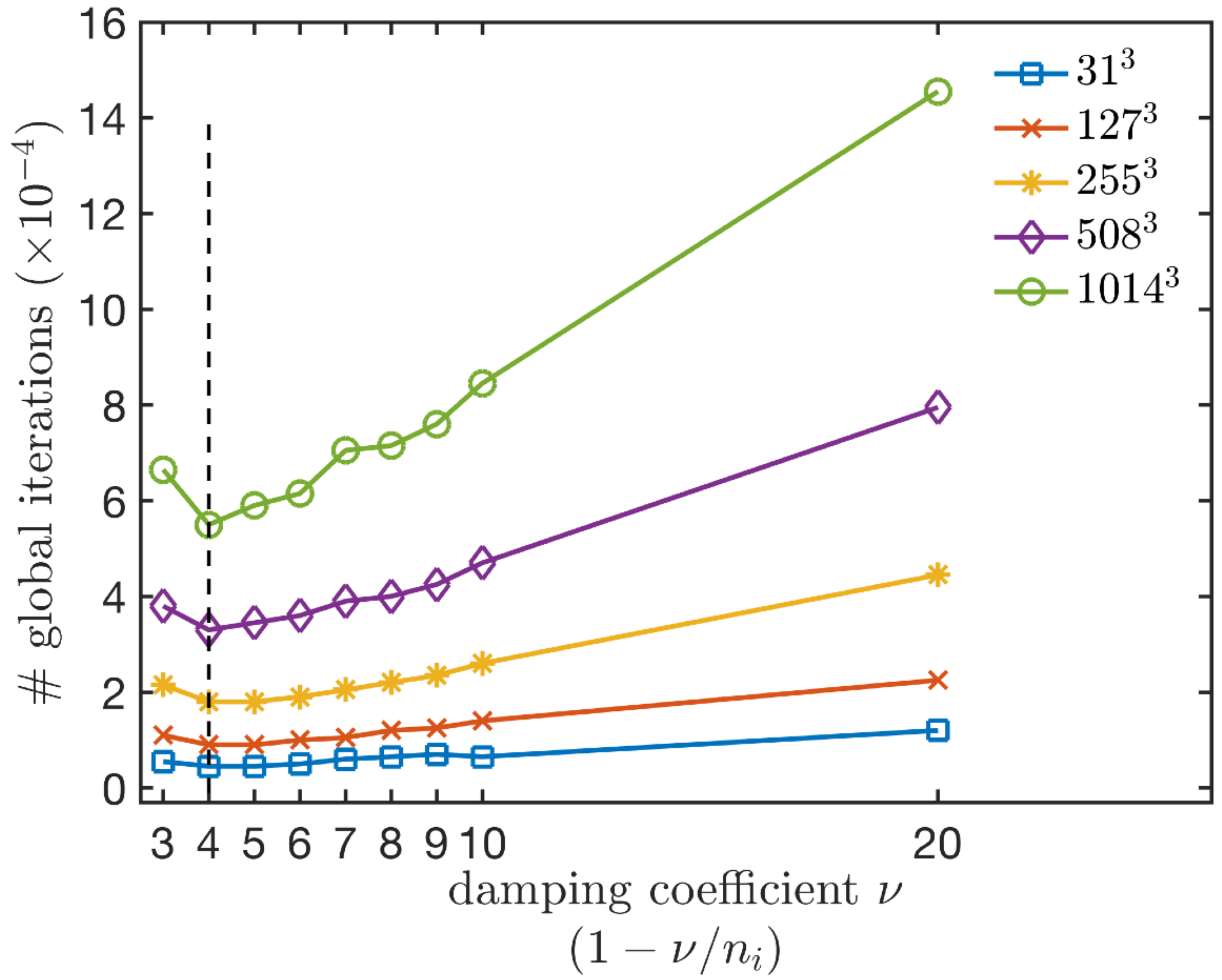


free parameter ν is resolution independent

Pseudo-Transient iterations

An improved approach

- Second order iterations: $$\alpha \cancelto{0}{\frac{\partial^2 A}{\partial \tau_{\mathrm{A}}^2}} + \cancelto{0}{\frac{\partial A}{\partial \tau_{\mathrm{A}}}} = f_{\mathrm{A}}$$

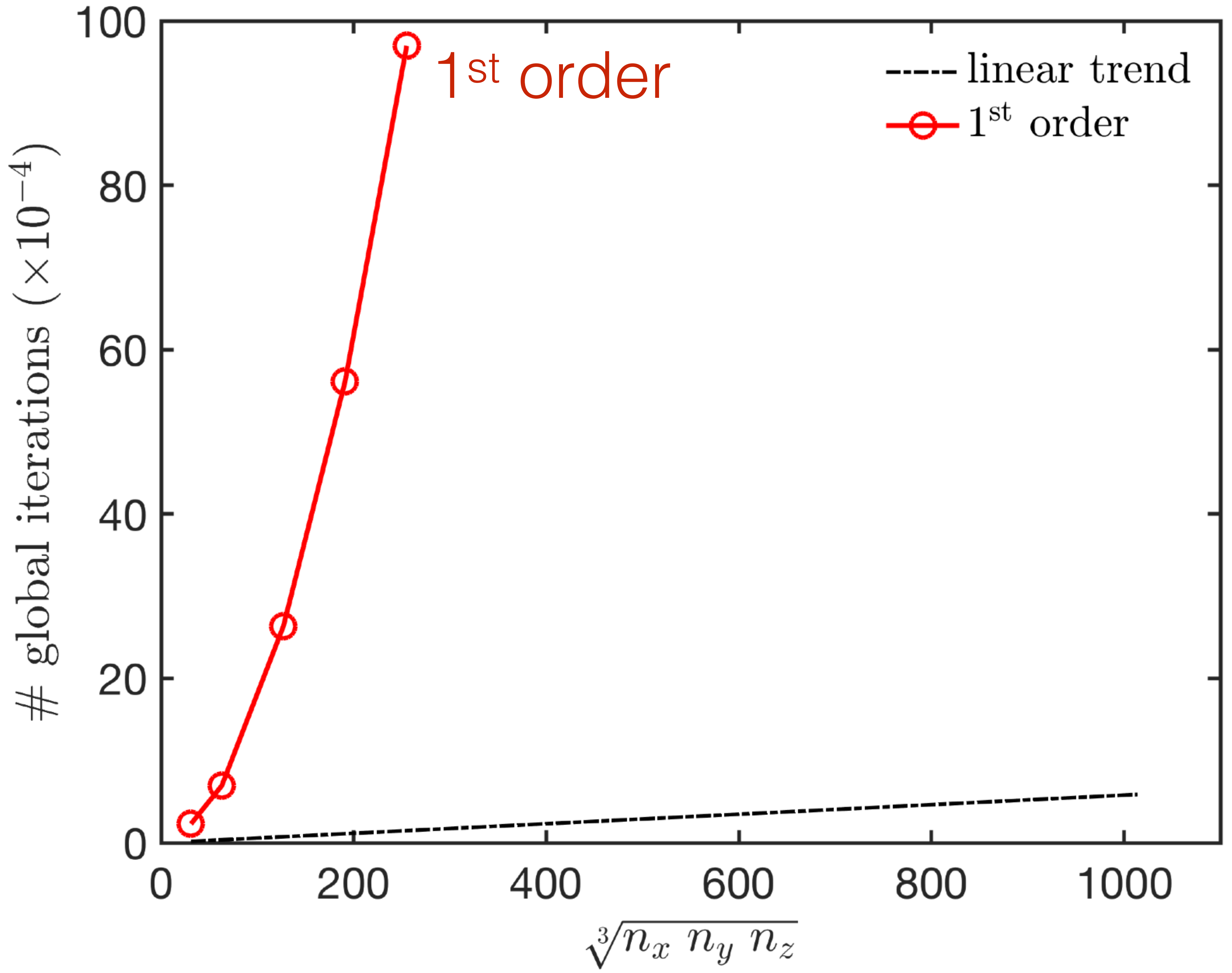
  Frankel, 1950

$$A^{[k+1]} = A^{[k]} + \Delta\tau_{\mathrm{A}} \left(\cancelto{0}{f_{\mathrm{A}}^{[k]}} + (1 - \nu/n_i)\, \cancelto{0}{f_{\mathrm{A}}^{[k-1]}} \right)$$ damping

- No global reduction: $\Delta\tau_{\mathrm{A}}$ is local (diagonal preconditionner)
- Only local communication: like propagation of physical information
- Same workflow on each grid point: perfect for GPUs !

Pseudo-Transient | improved

- 1^{st} versus 2^{nd} order scheme | 3-D hydro-mechanics



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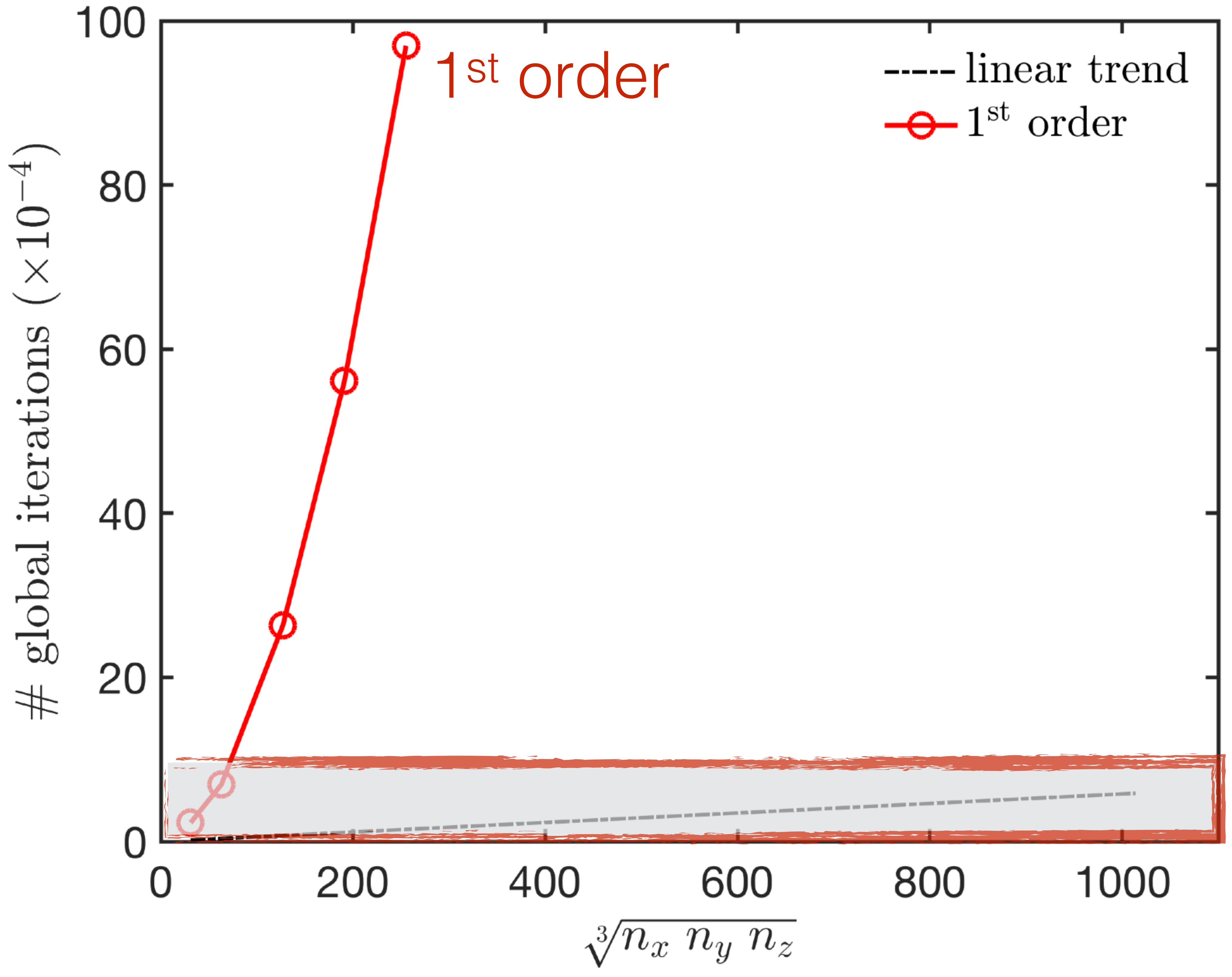

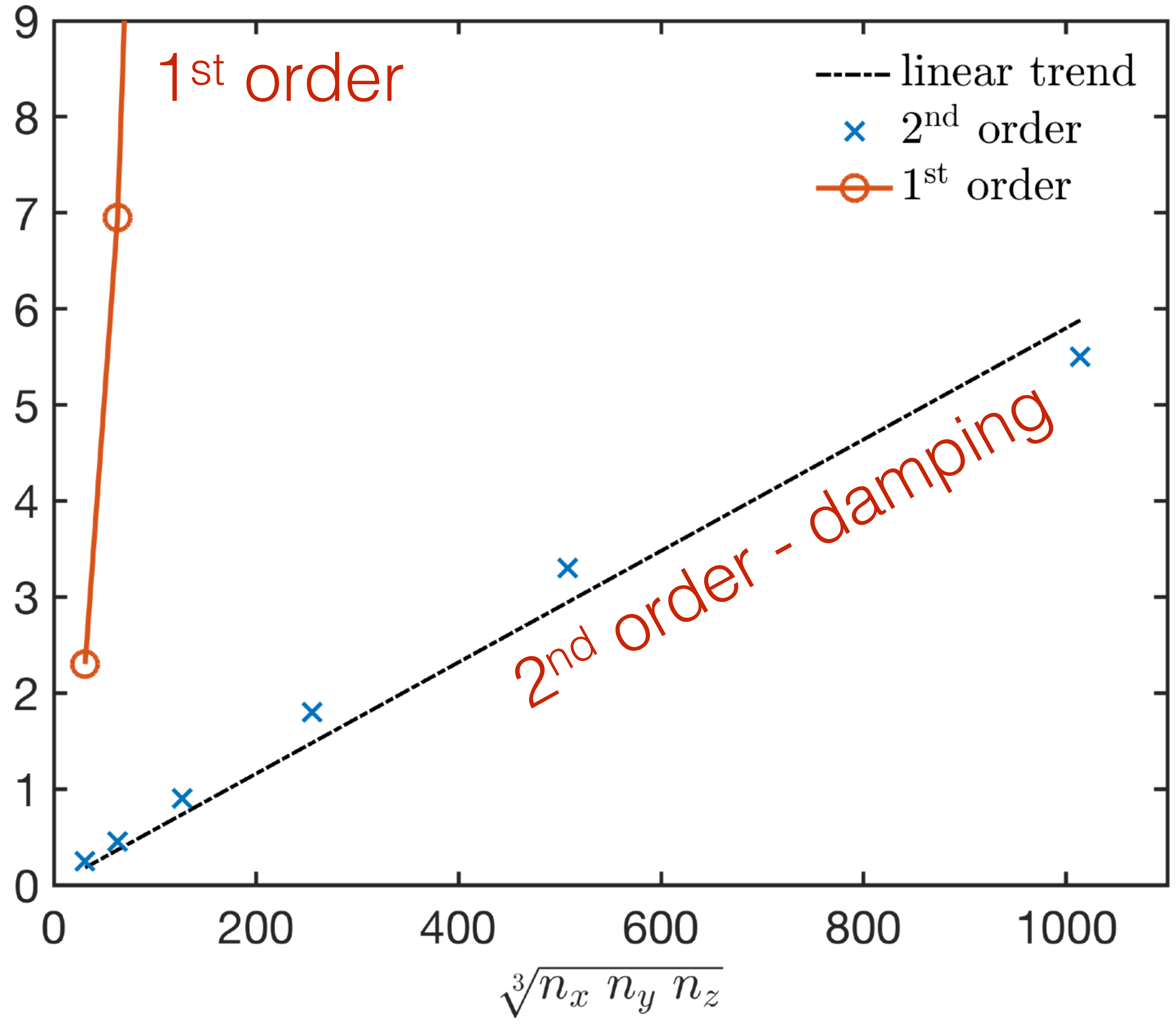

Pseudo-Transient | improved

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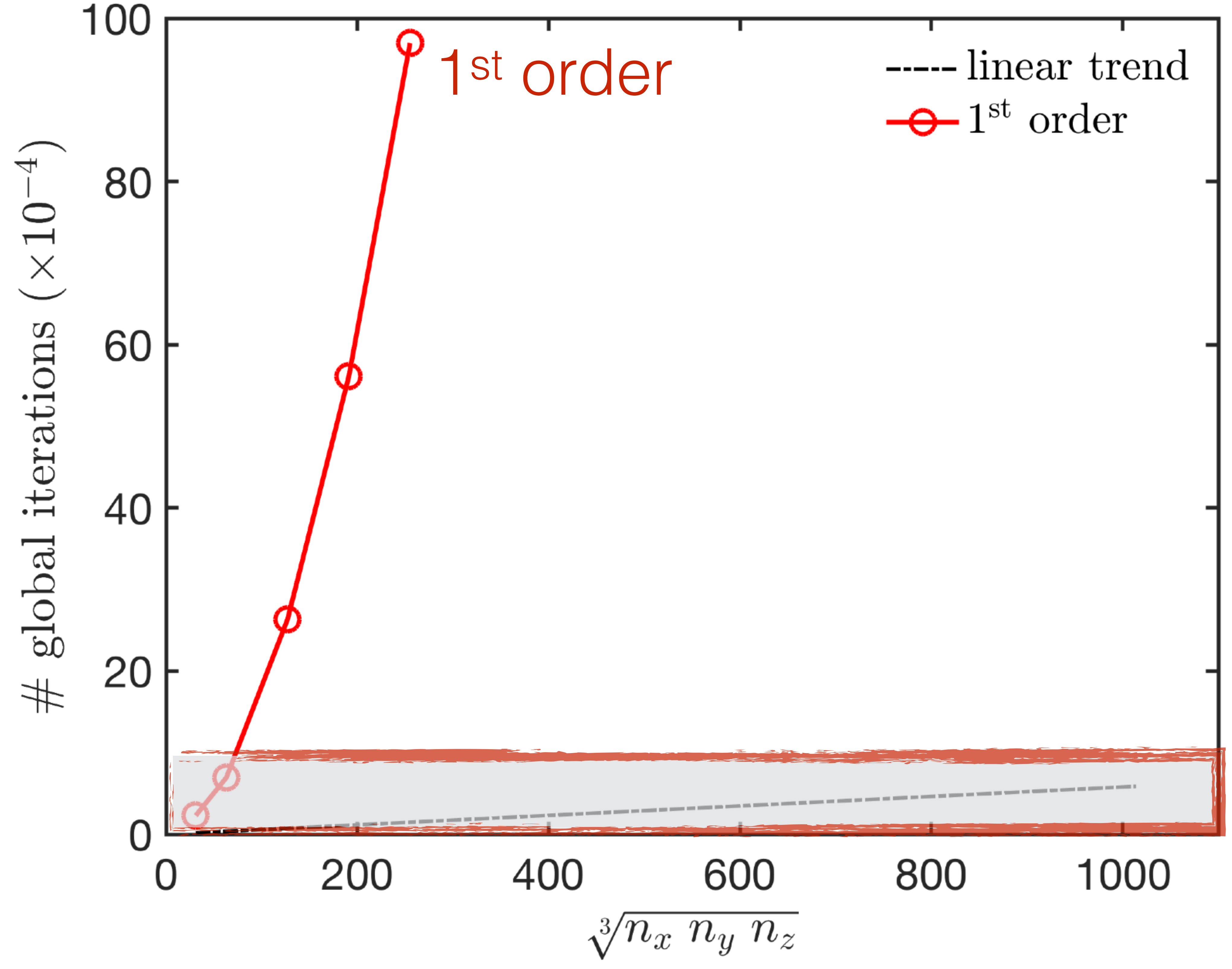
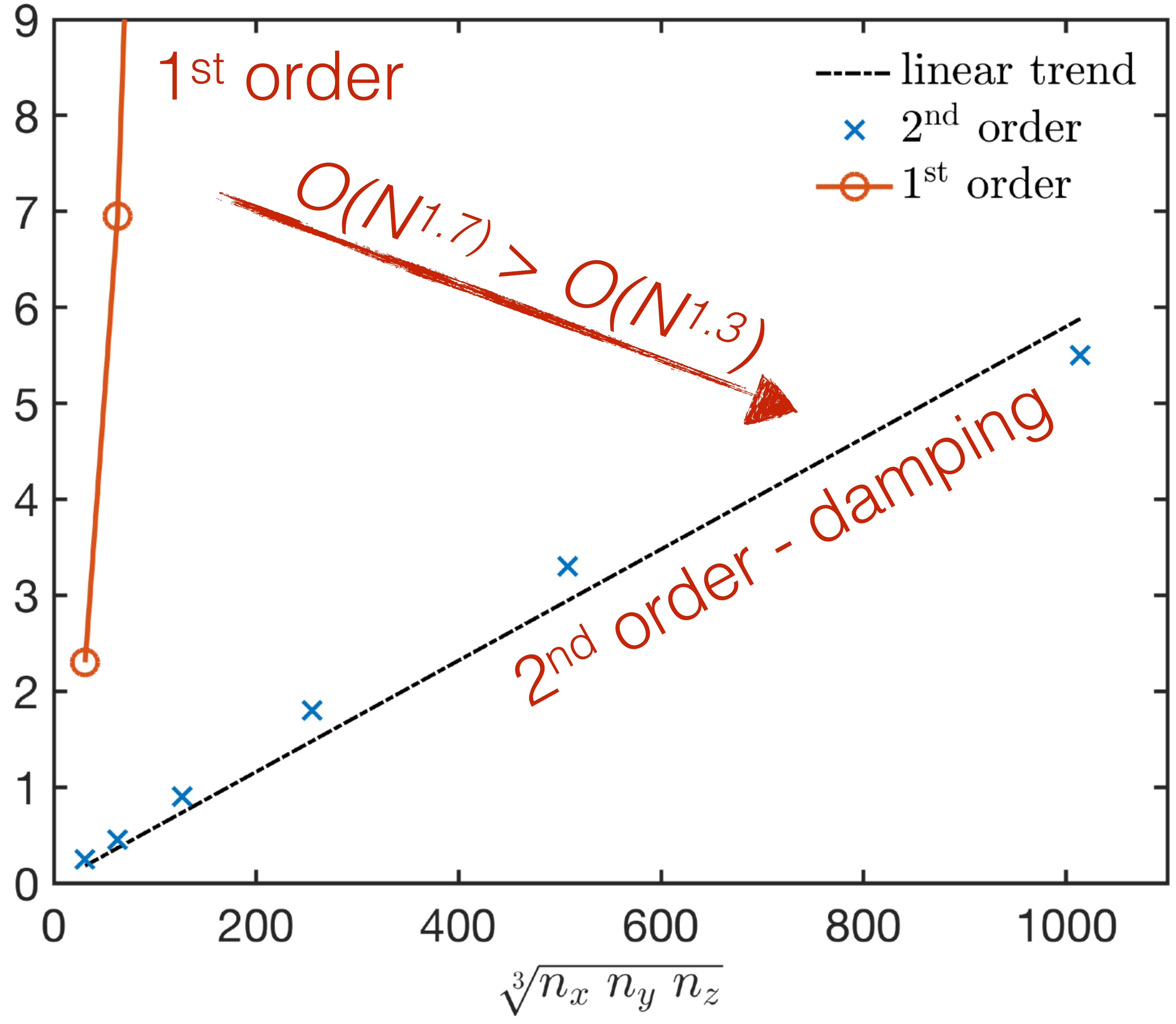
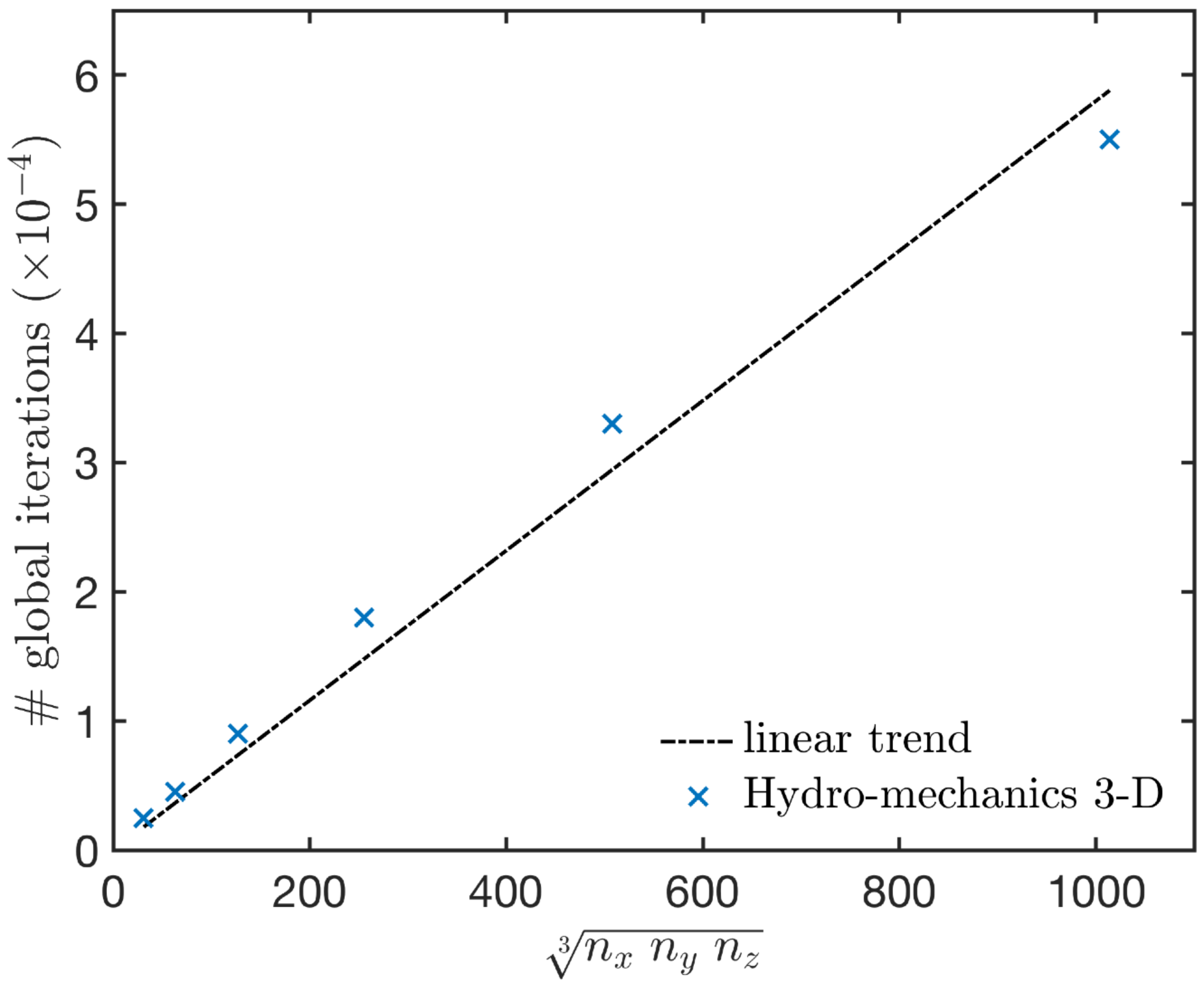
Yay! Scales $O(N^{1.3})$





Iteration count ≠ time to solution

- Comparison to algorithms with ideal scalability



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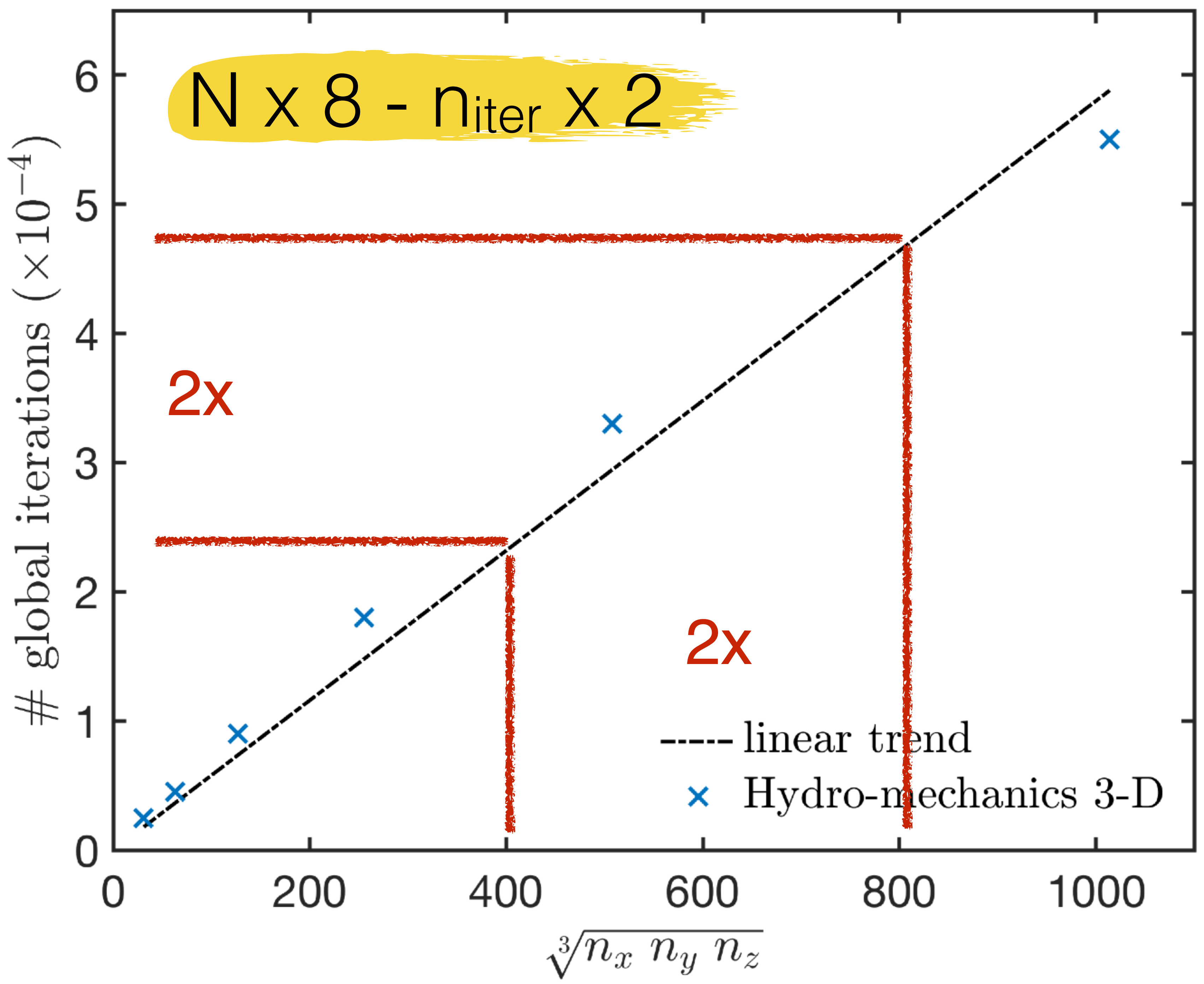

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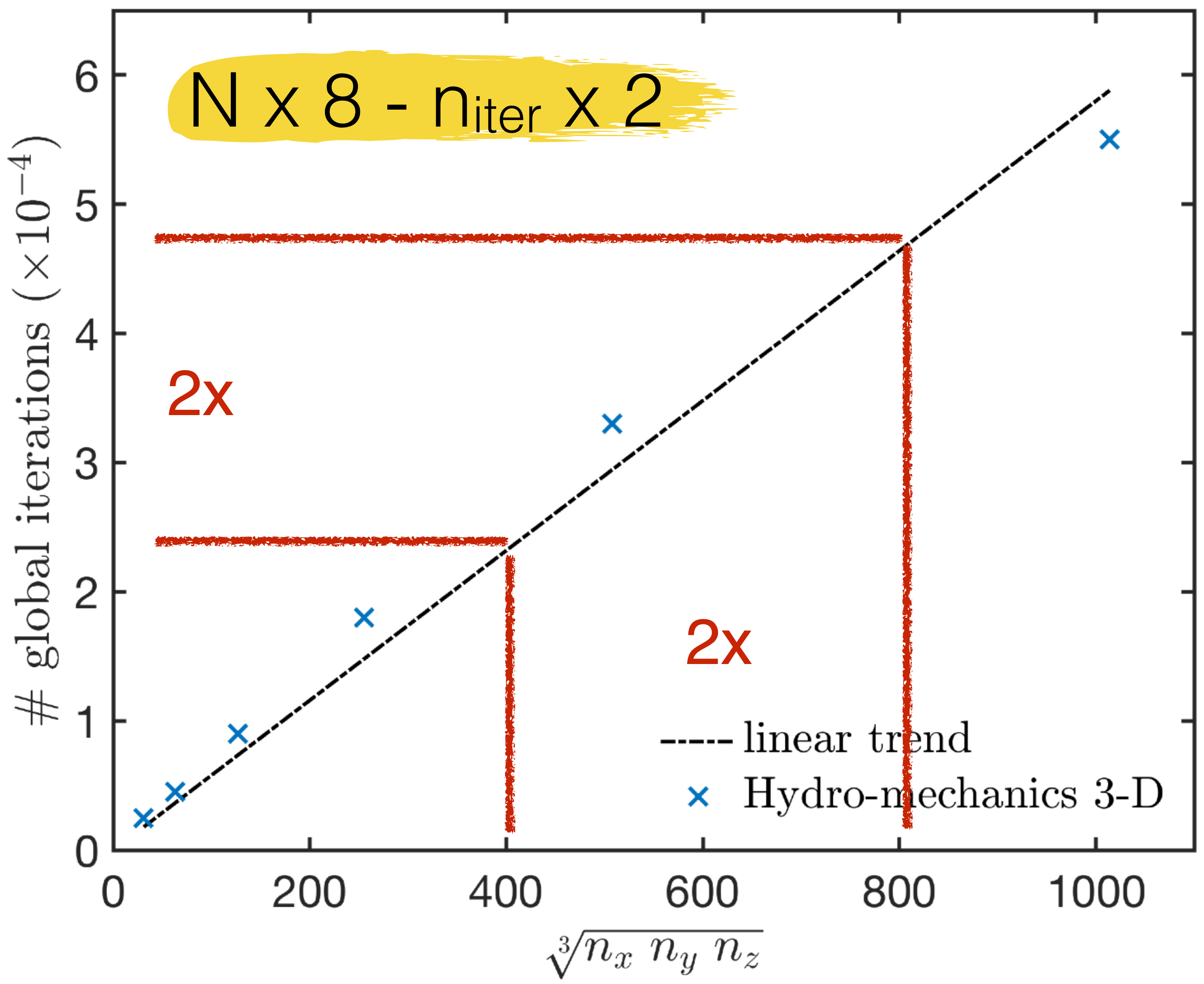

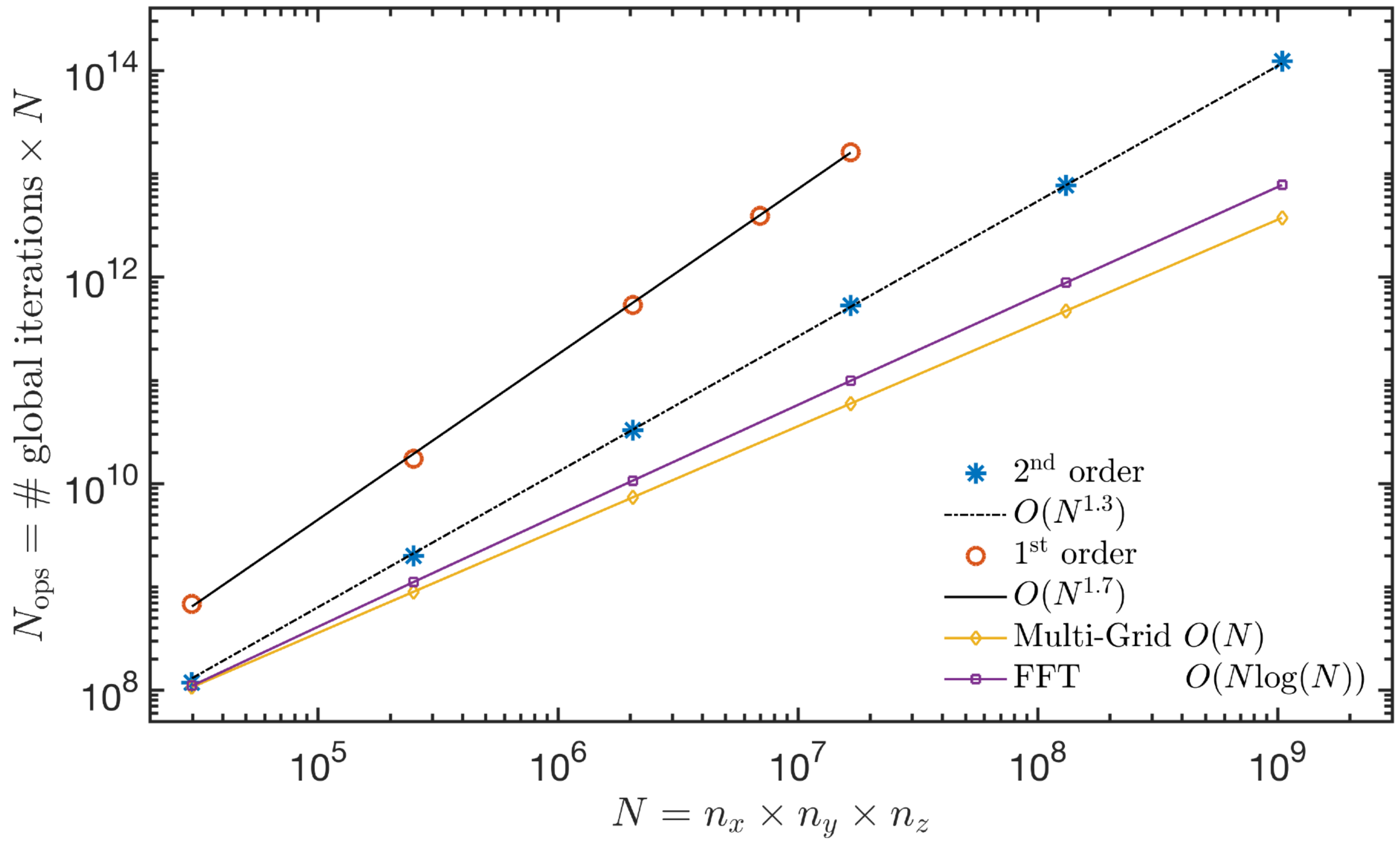

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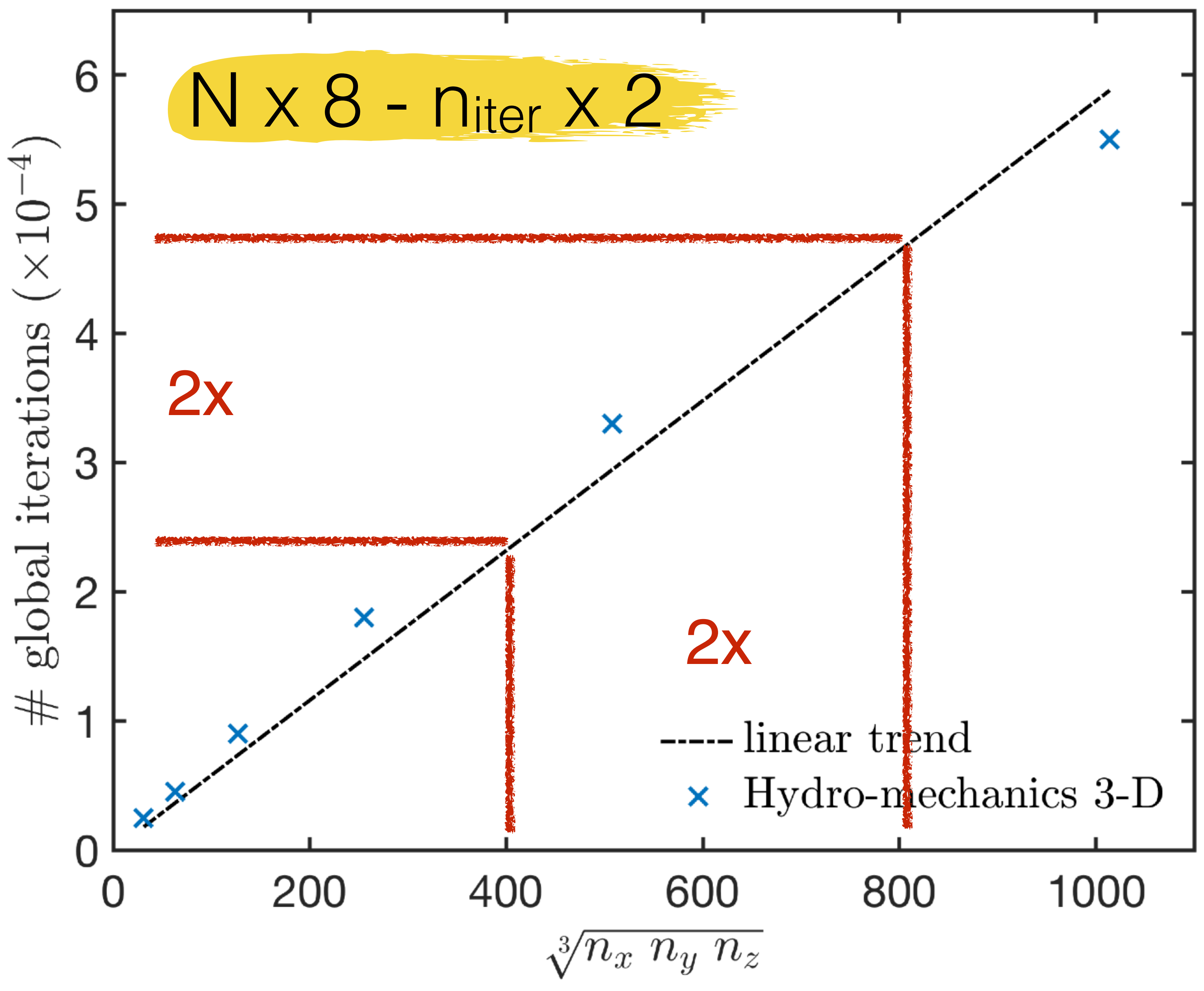

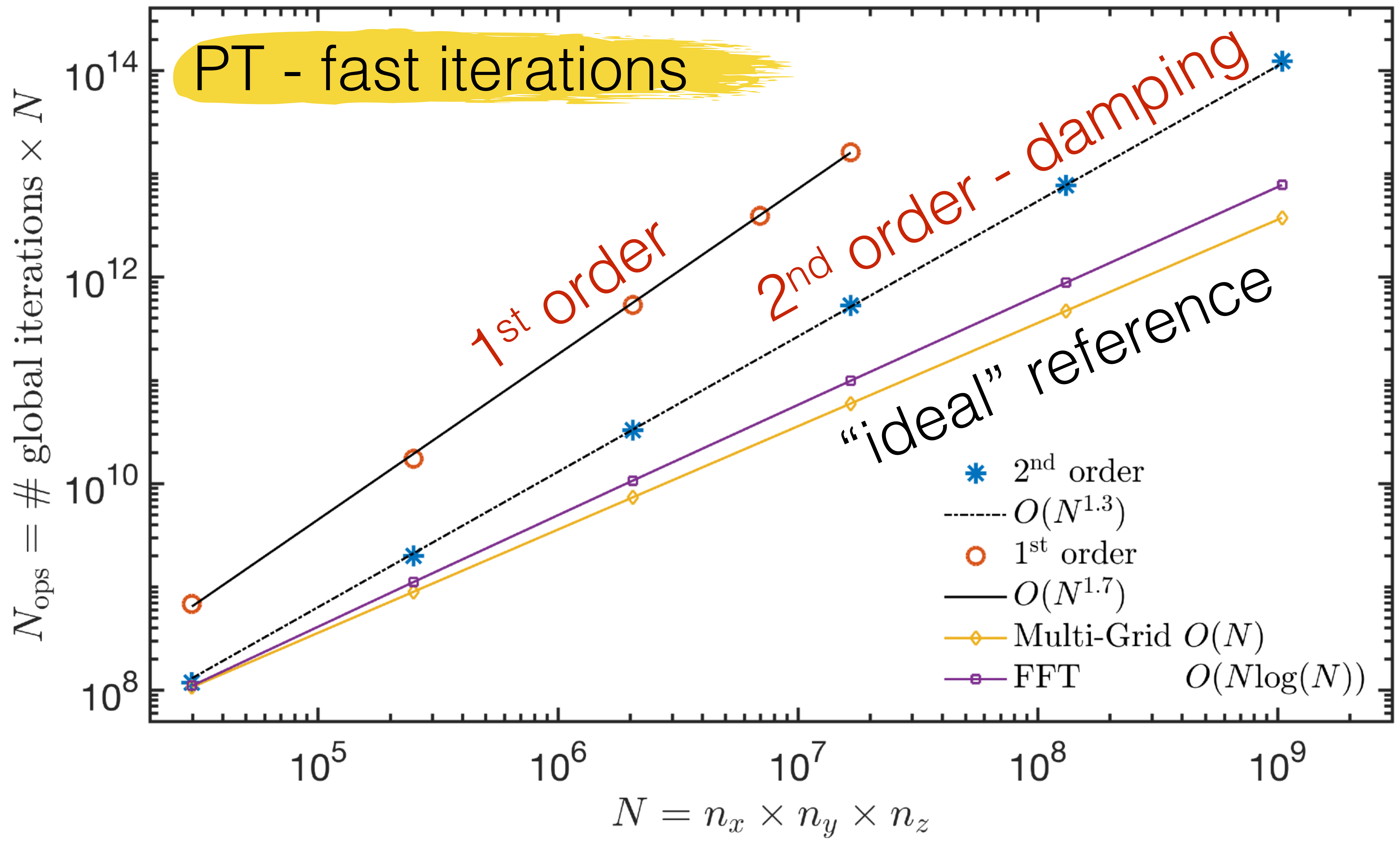

1/ Pseudo-Transient

Summary

- Pseudo-transient brings back transient physics and converges fast: $O(N^{1.3})$
- Second order - no additional communication (still local)
- But … additional memory transfers (past residual field [k-1] - damping)
- No need to gather information across the entire domain

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Summary

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- Second order - no additional communication (still local)
- But … additional memory transfers (past residual field [k-1] - damping)
- No need to gather information across the entire domain

Physics is local & parallel - like nature

2/ Parallel efficiency

Distributed memory | large 3-D problem does not fit in a single GPU memory

- MPI: domain decomposition
- Send boundary points to neighbours as B.C.
- 6 planes to send in 3-D per sub-domain
- Volume to area ratio is the killer in 3-D
- Parallel efficiency will drop with more procs

  - network congestion, many HPC users, …

Conceptual 2-D domain decomposition

2/ Parallel efficiency

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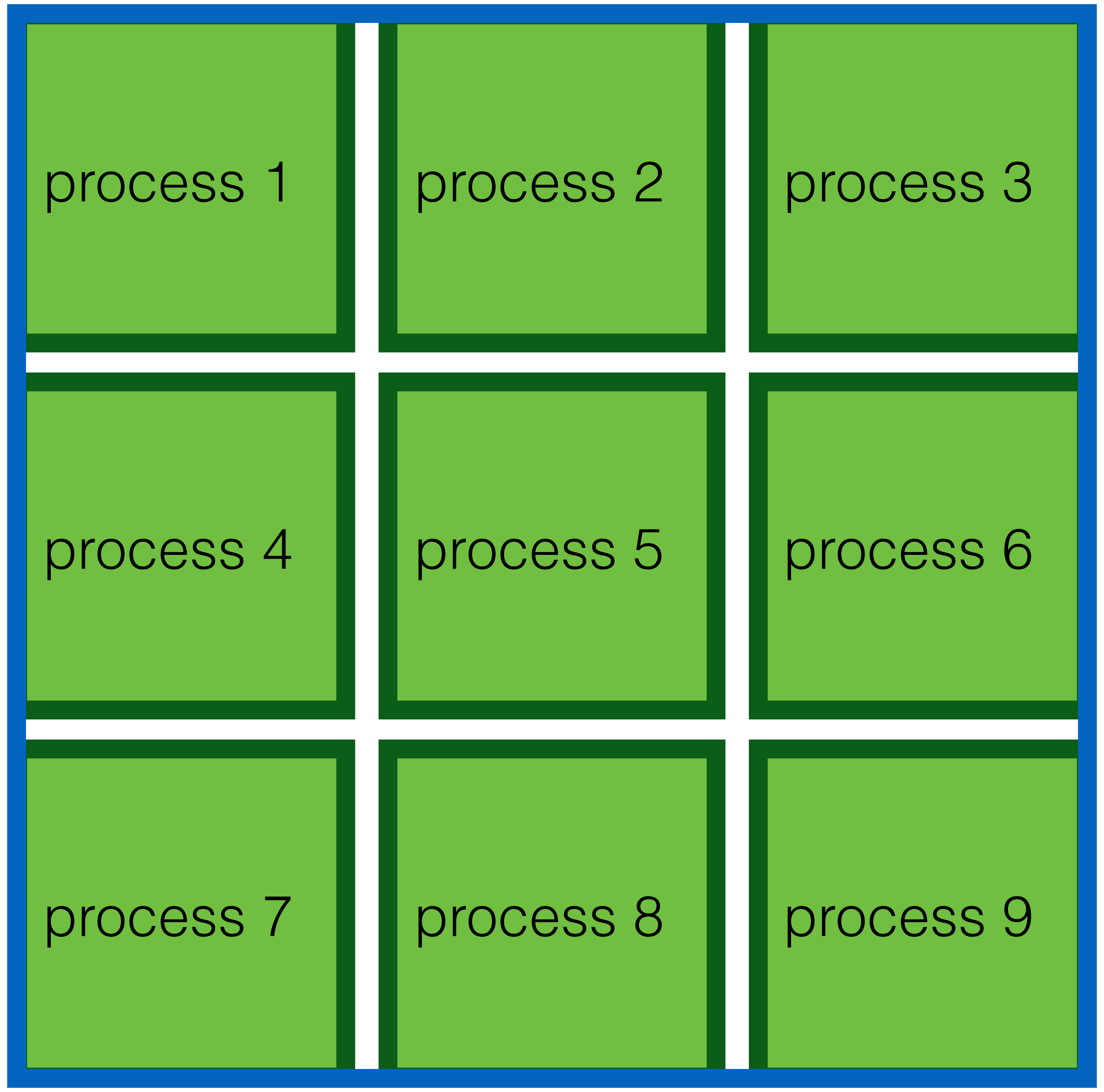
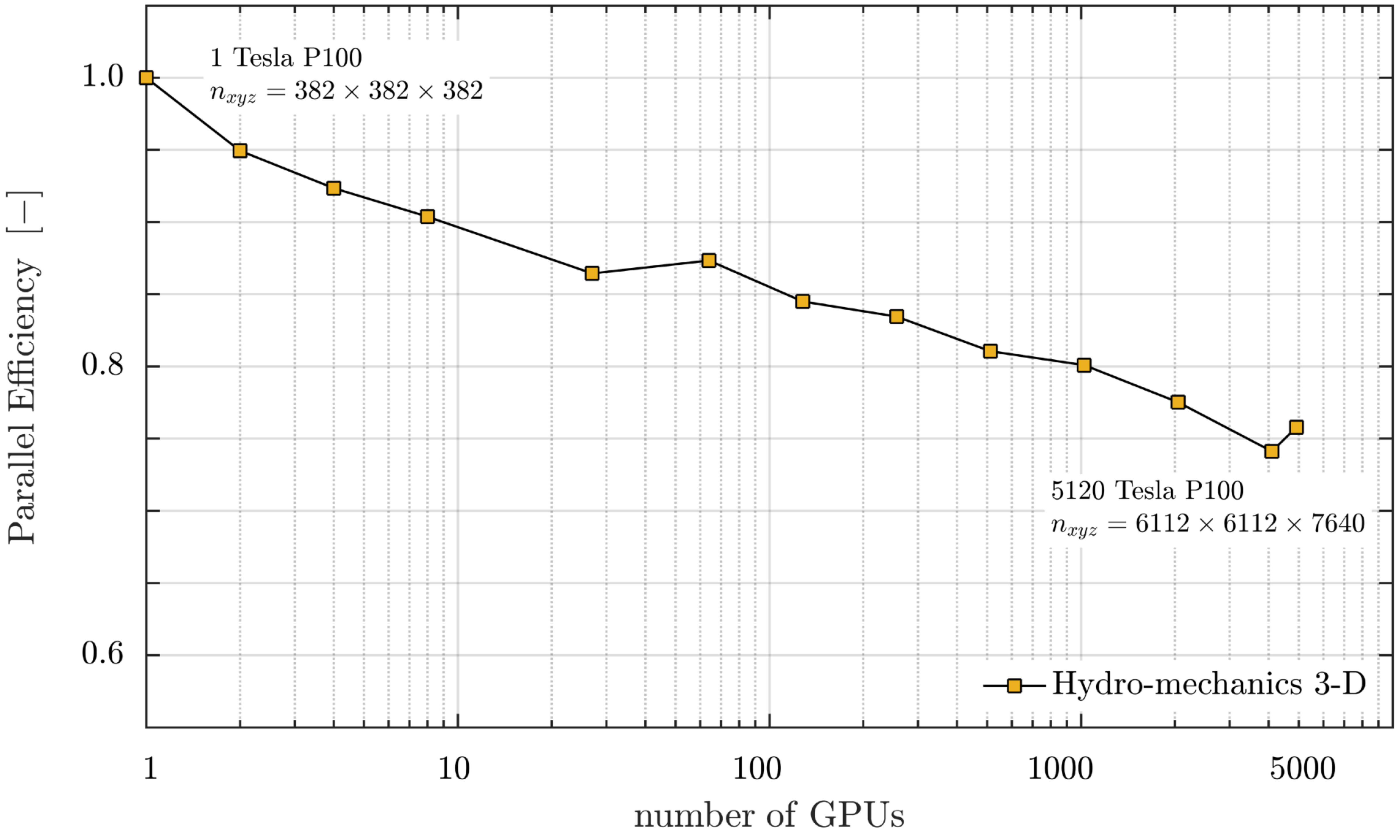


Costs of communication increase

- What will naively happen (weak scaling - physics efficiency = 1)



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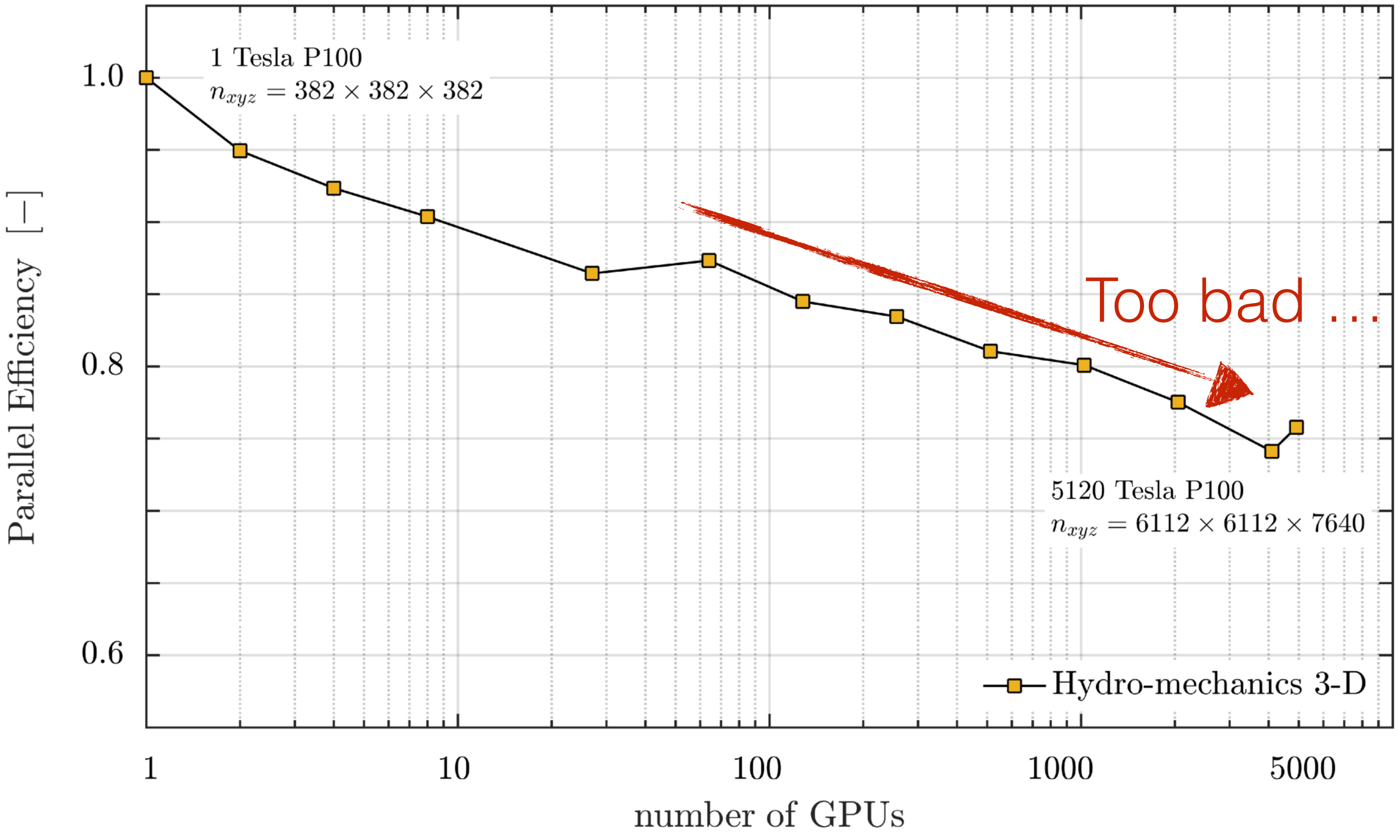

Costs of communication increase

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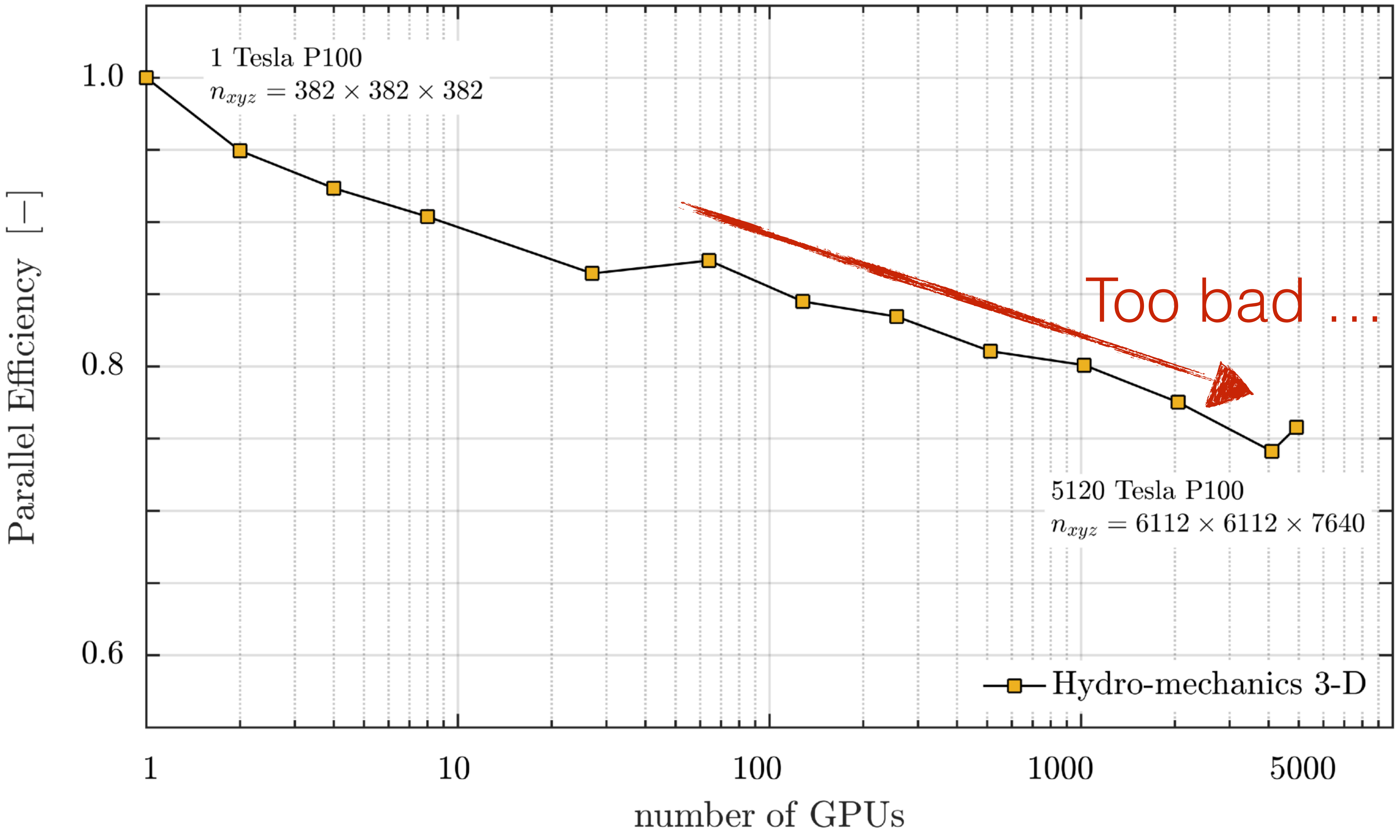
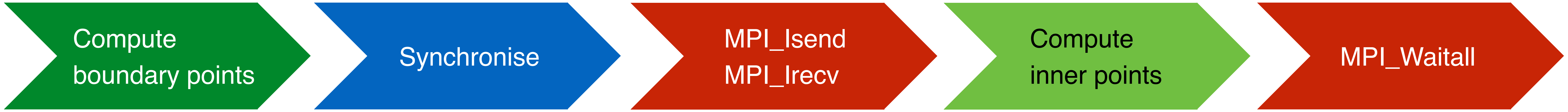
Solution: hide MPI communication

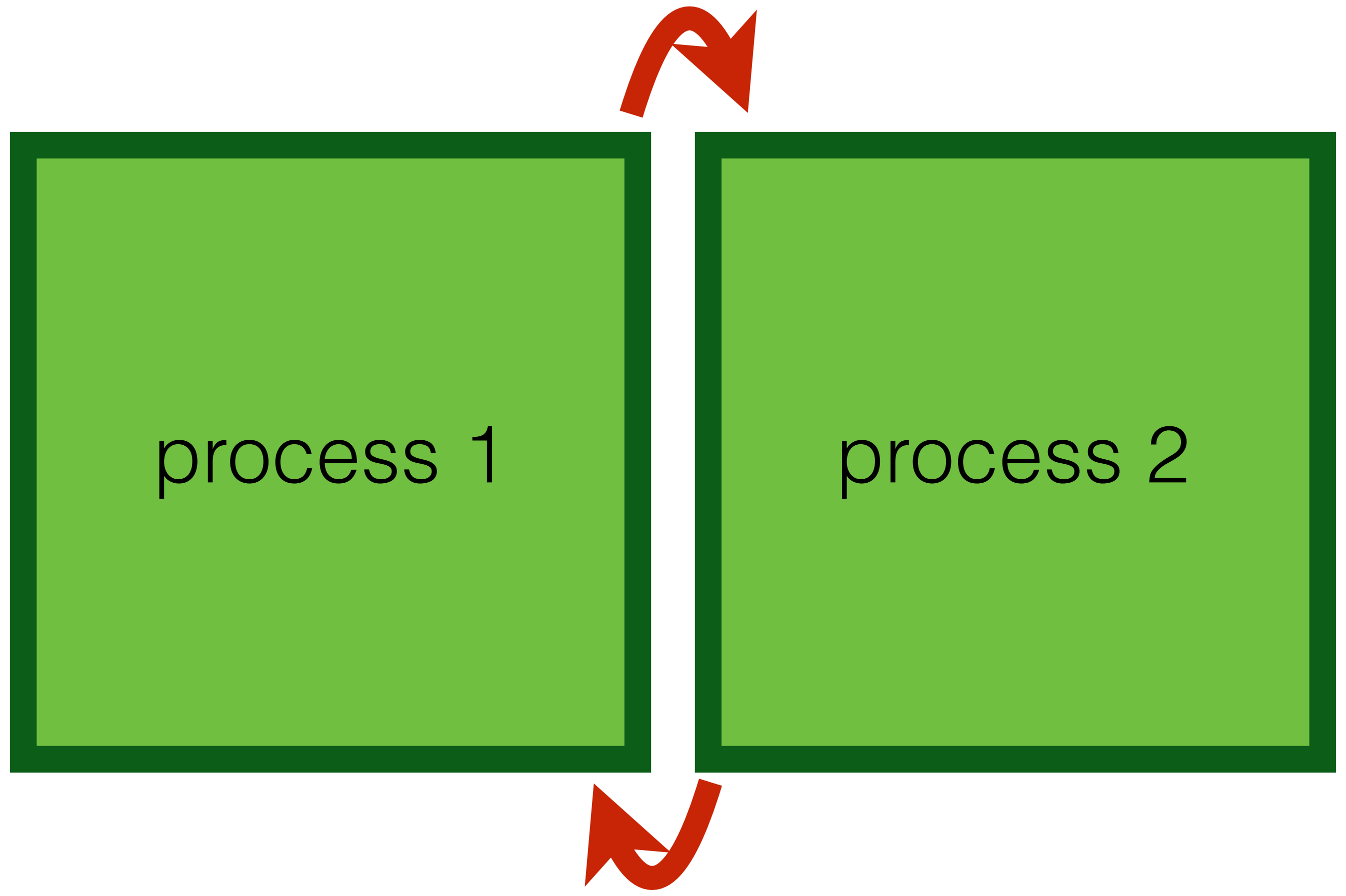


Hiding communication

- The simple concept:

Overlap boundary node communication with inner points computations





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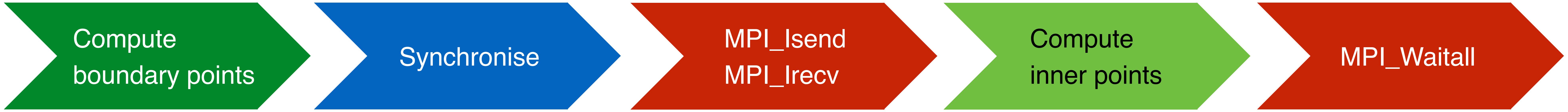

Conceptually simple, but no “easy solution” for real-world applications

Hiding communication

- The simple concept:

Overlap boundary node communication with inner points computations

MPI message progression in background will not continue
Need e.g. to call MPI_test to keep it alive … [1]

[1] *Hoefler and Lumsdaine, 2008. IEEE on cluster comp.*

Hiding communication

- The simple concept:

Overlap boundary node communication with inner points computations

MPI message progression in background will not continue
Need e.g. to call MPI_test to keep it alive … [1]

- The “MPI_test” approach may be complicated to do for a real world application...

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Hiding communication

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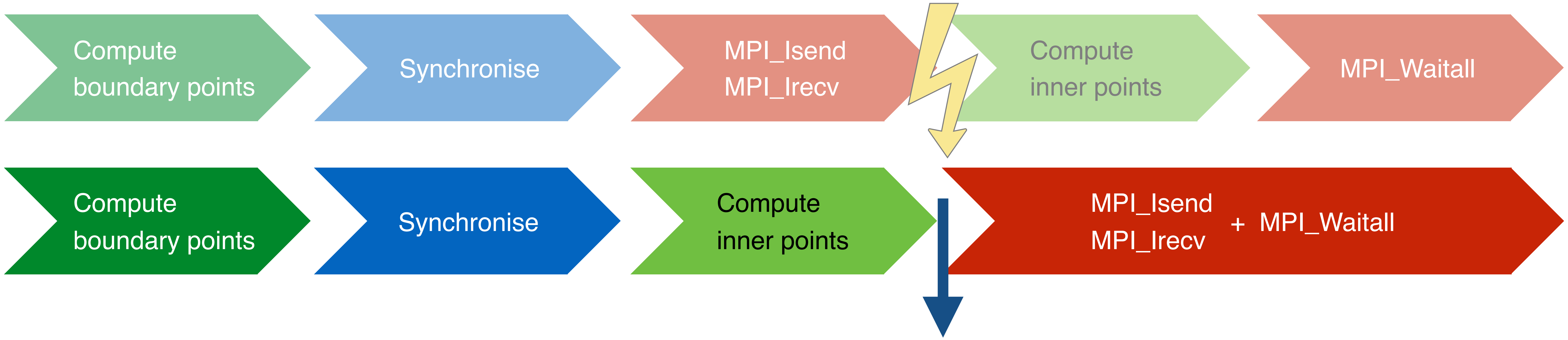
Overlap boundary node communication with inner points computations



Control goes back to host thread, next step begins directly.
The host threads blocks only when reaching MPI_Waitall:
> trivially ensures persistent message progression (basic MPI)

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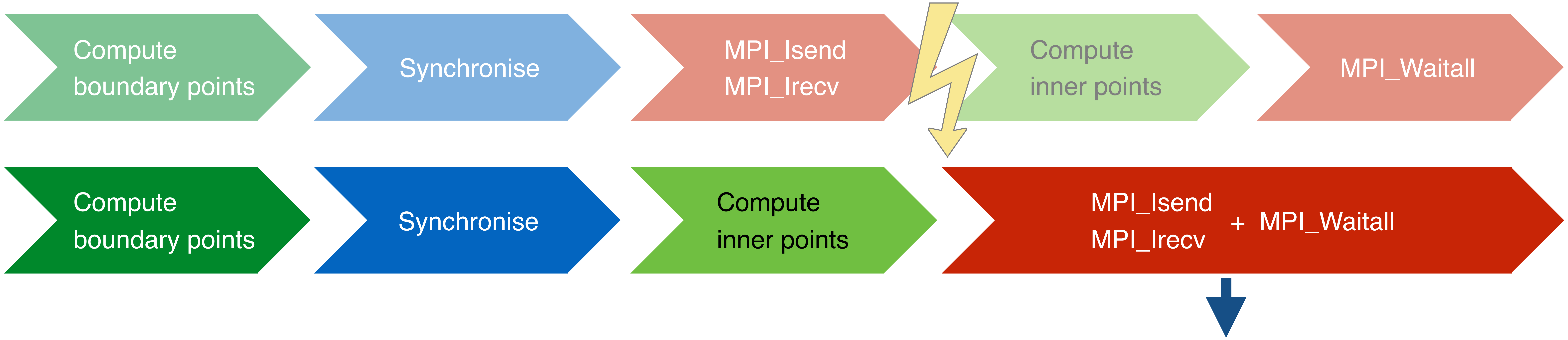

Synchronise + call MPI_Waitall freely in this function

/!\ Only avoid blocking the GPU kernel [Compute inner points] !

Hiding communication

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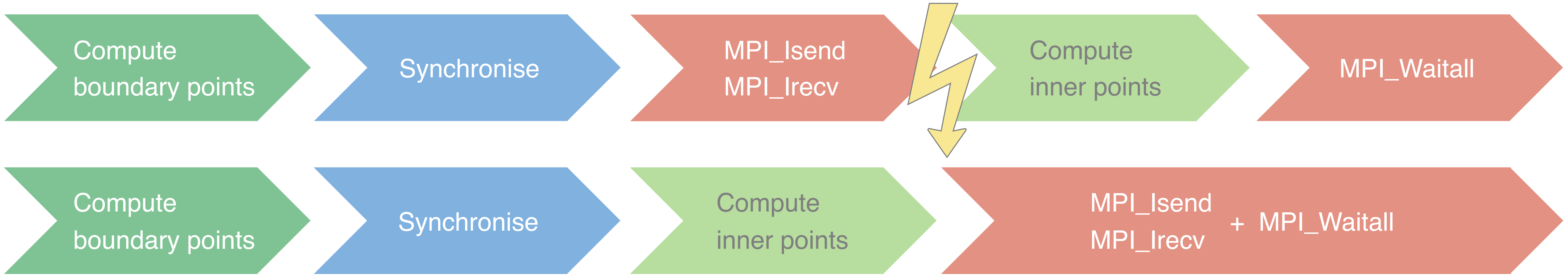
Overlap boundary node communication with inner points computations



- How to access boundary data on the GPU without blocking the ongoing computations ?
- How to make this fast in order to quickly initiate the MPI data transfers ?

Hiding communication

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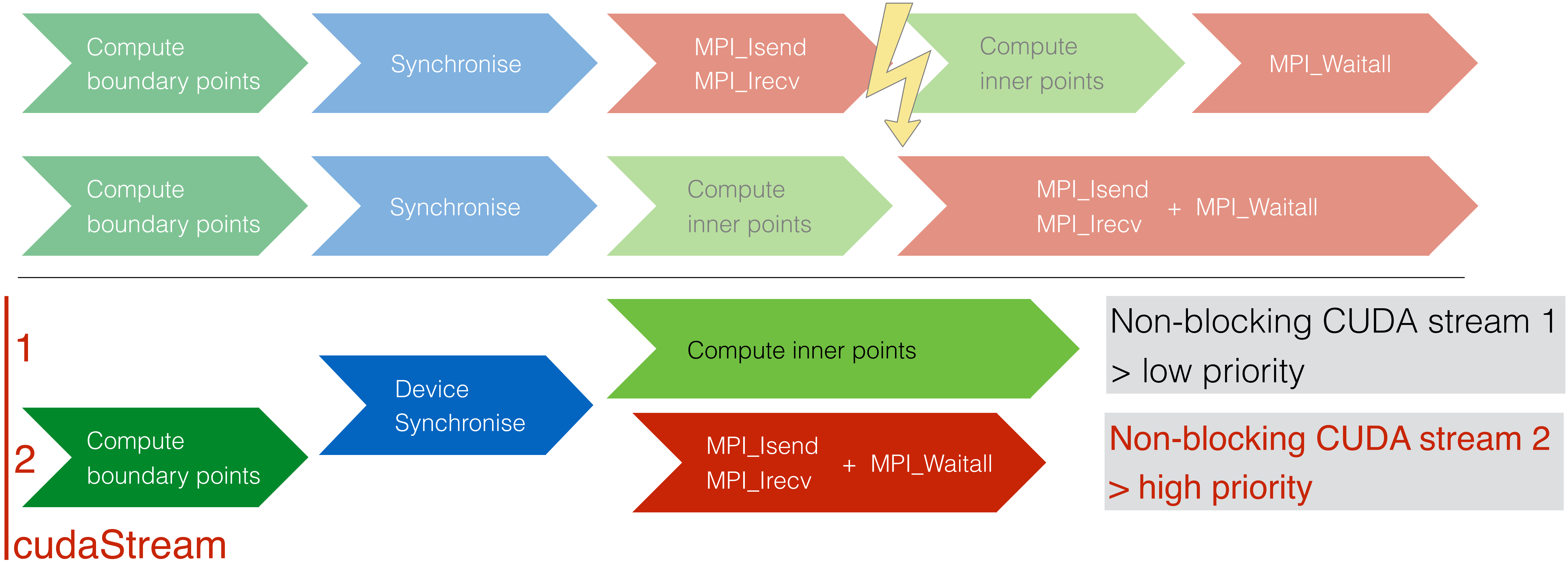
Overlap boundary node communication with inner points computations

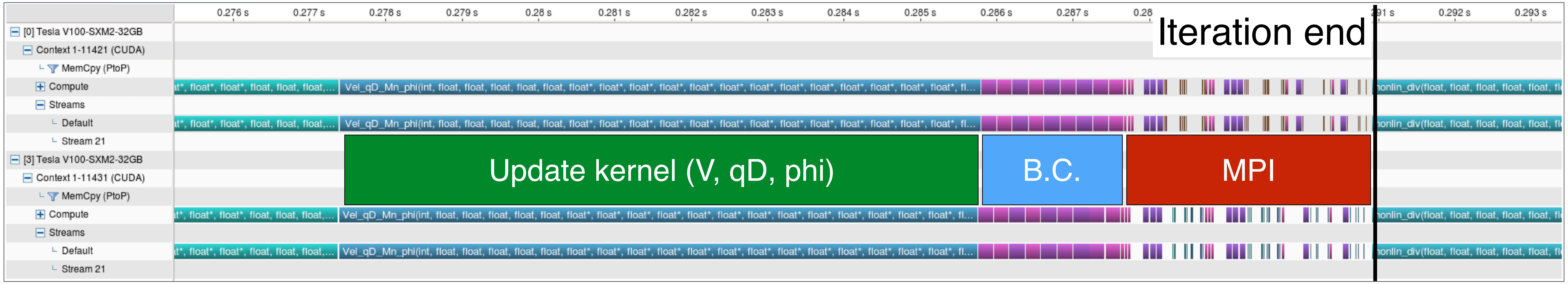


Visual profiler (nvvp)

Original

Visual profiler (nvvp)

Original



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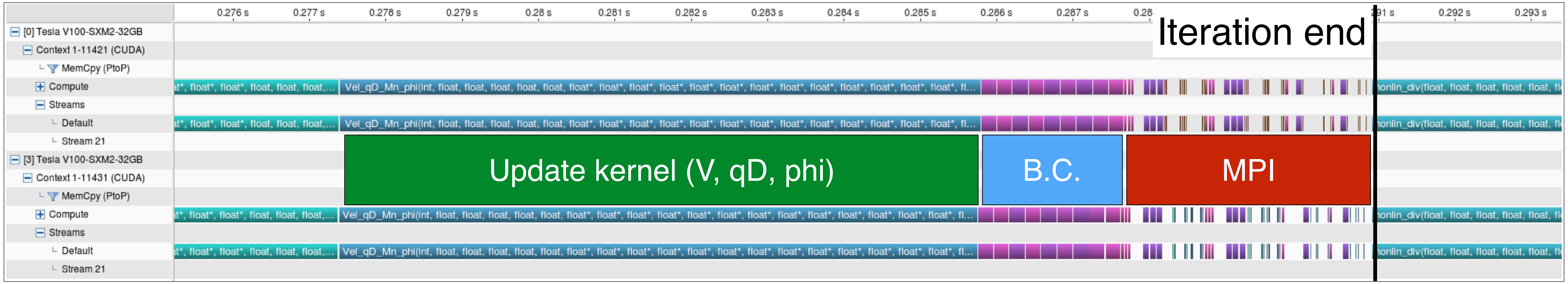
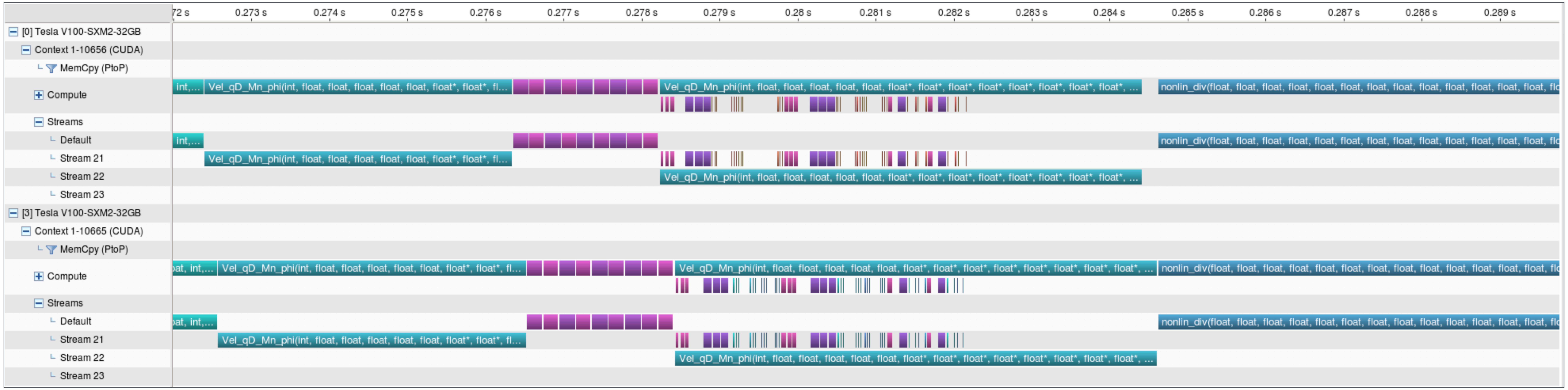


Hide MPI



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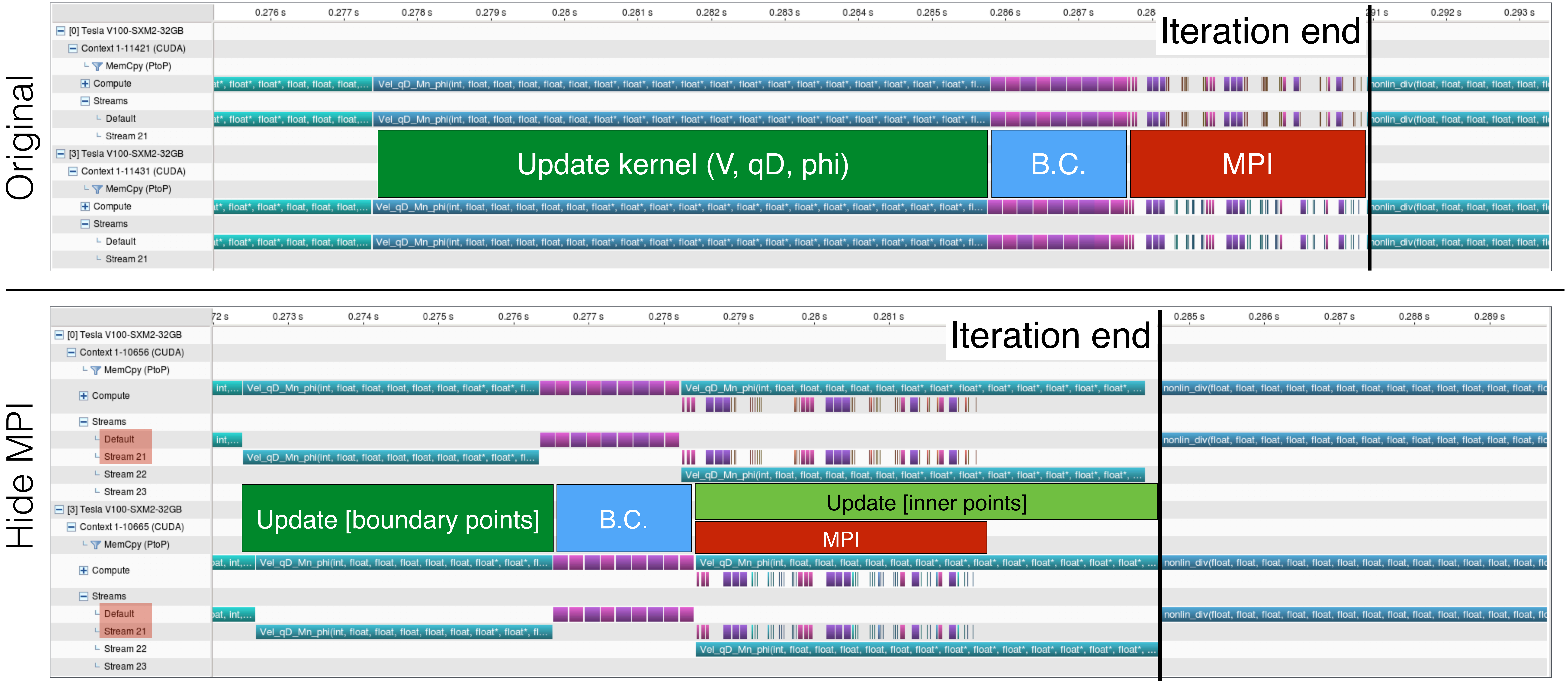

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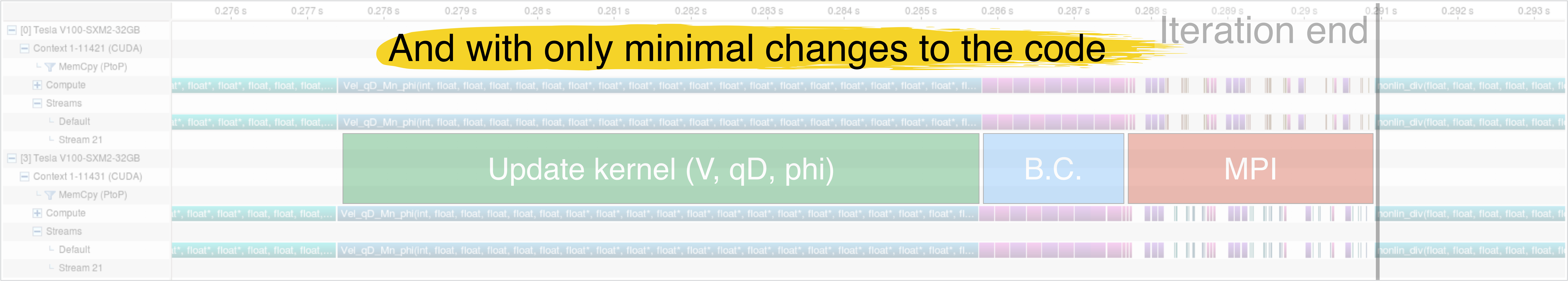

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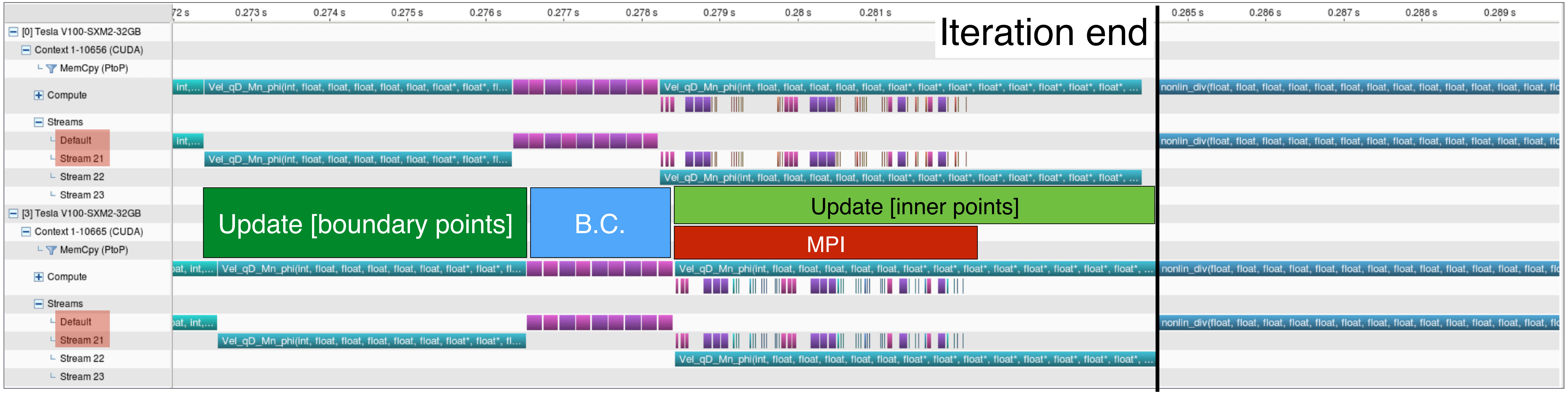

Minimal changes to the code

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__global__ void compute(int istep){
    int ix = blockIdx.x*blockDim.x + threadIdx.x; // thread ID, dimension x
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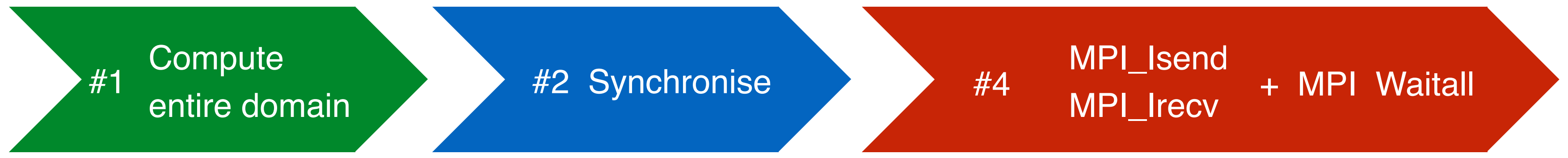
    int iz = blockIdx.z*blockDim.z + threadIdx.z; // thread ID, dimension z

    //(...) (rest of the kernel as before)
}

main(){
    //(...)

        compute<<<grid,block                 >>>(      );     // step 1
                    cudaDeviceSynchronize();                   // step 2

    update_boundaries();                                       // step 4
    //(...)
}
```



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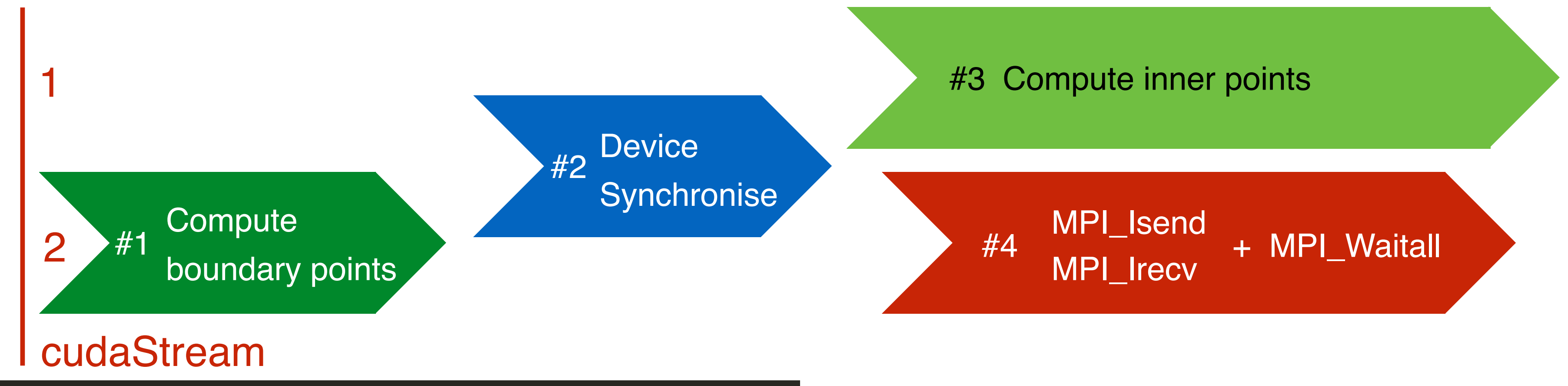
    }
    update_boundaries();                                      // step 4
    //(...)
}
```



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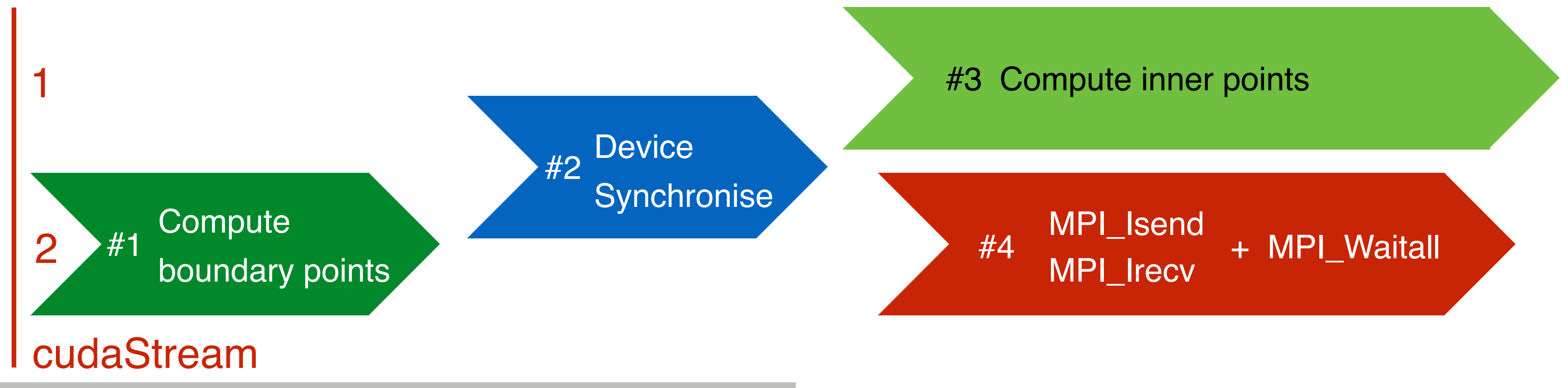
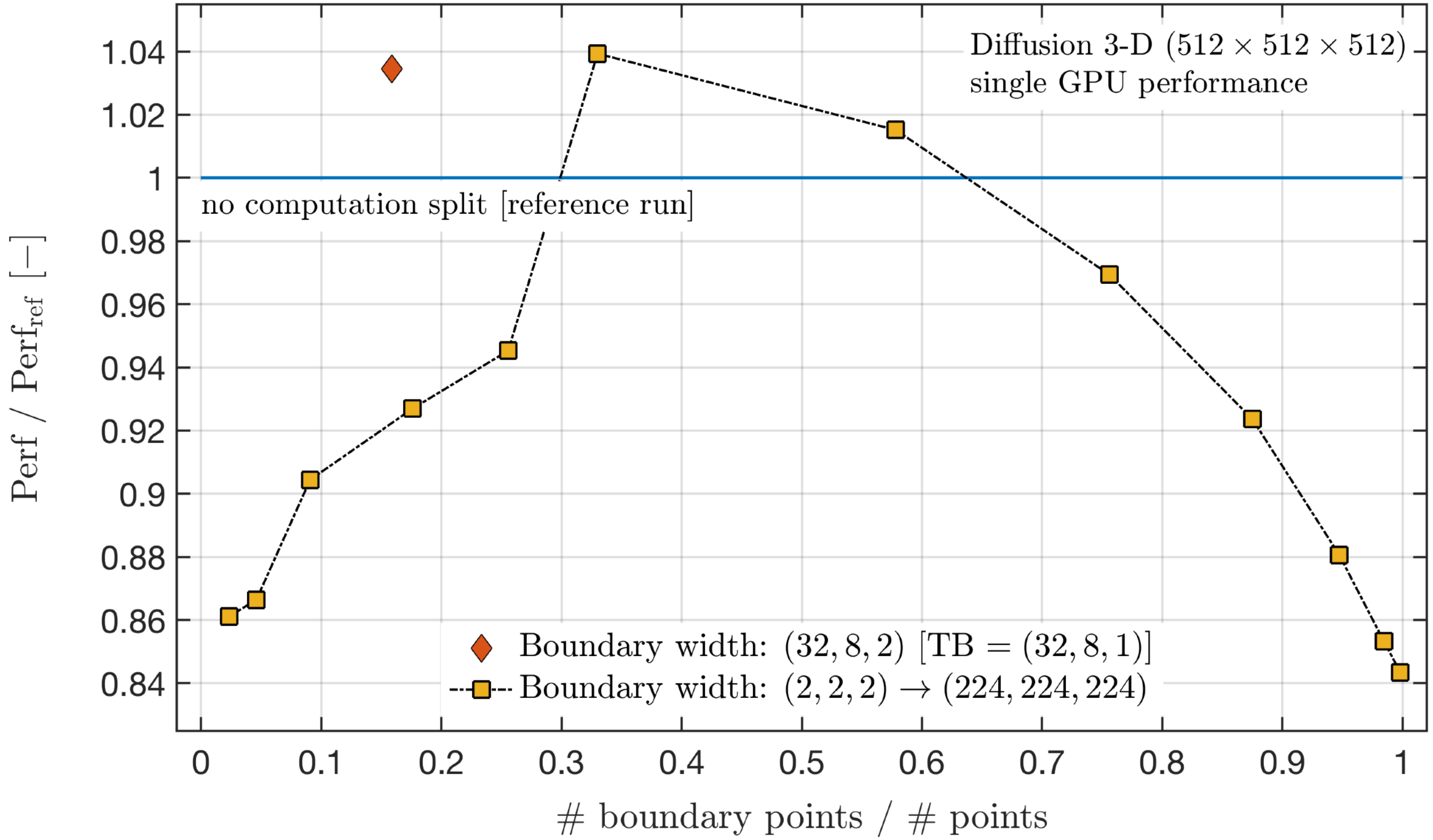


Avoid loss of performance when splitting boundary: Make boundary width > 2

Avoid loss of performance

- Impact of boundary width on single GPU performance



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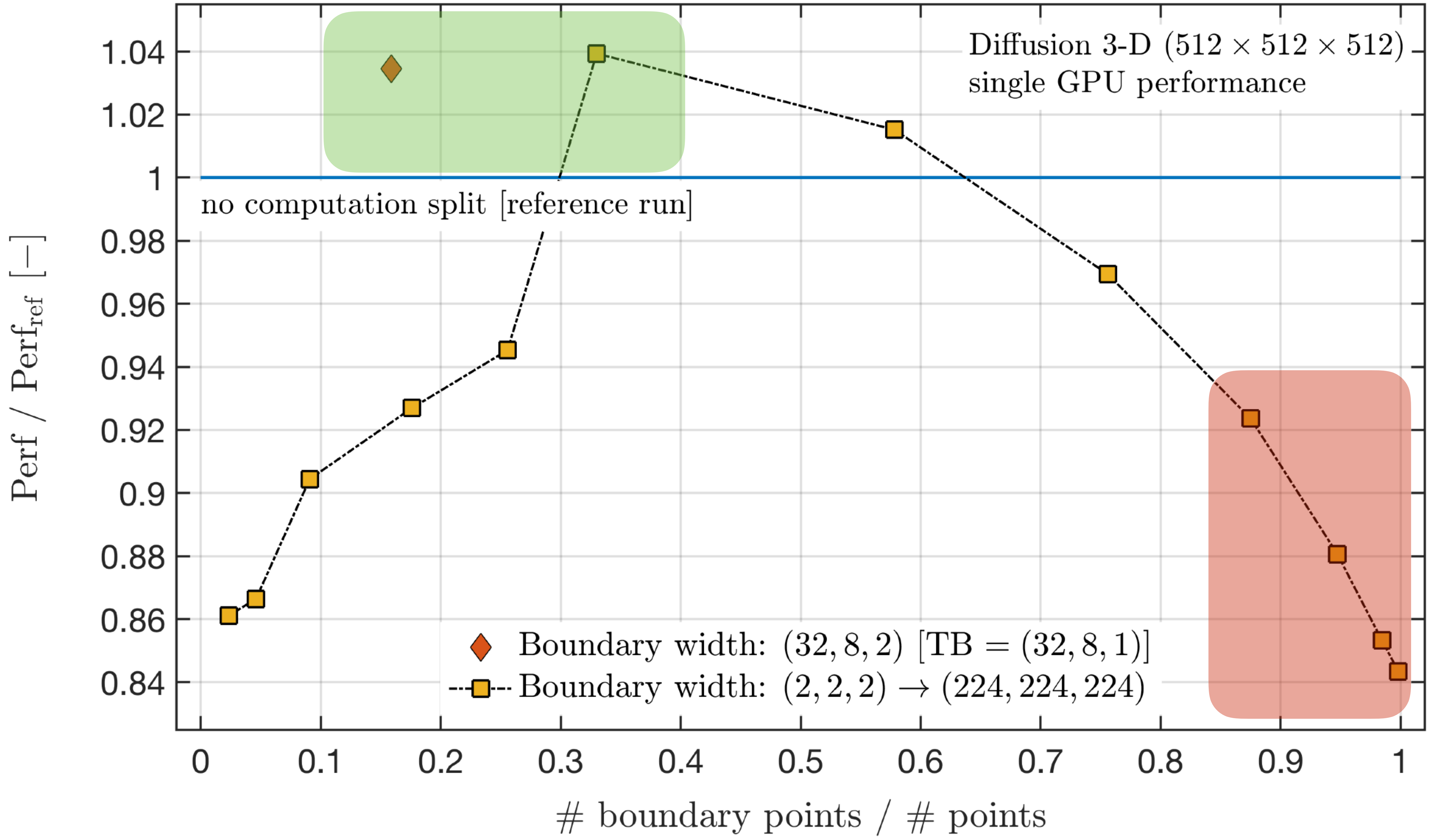

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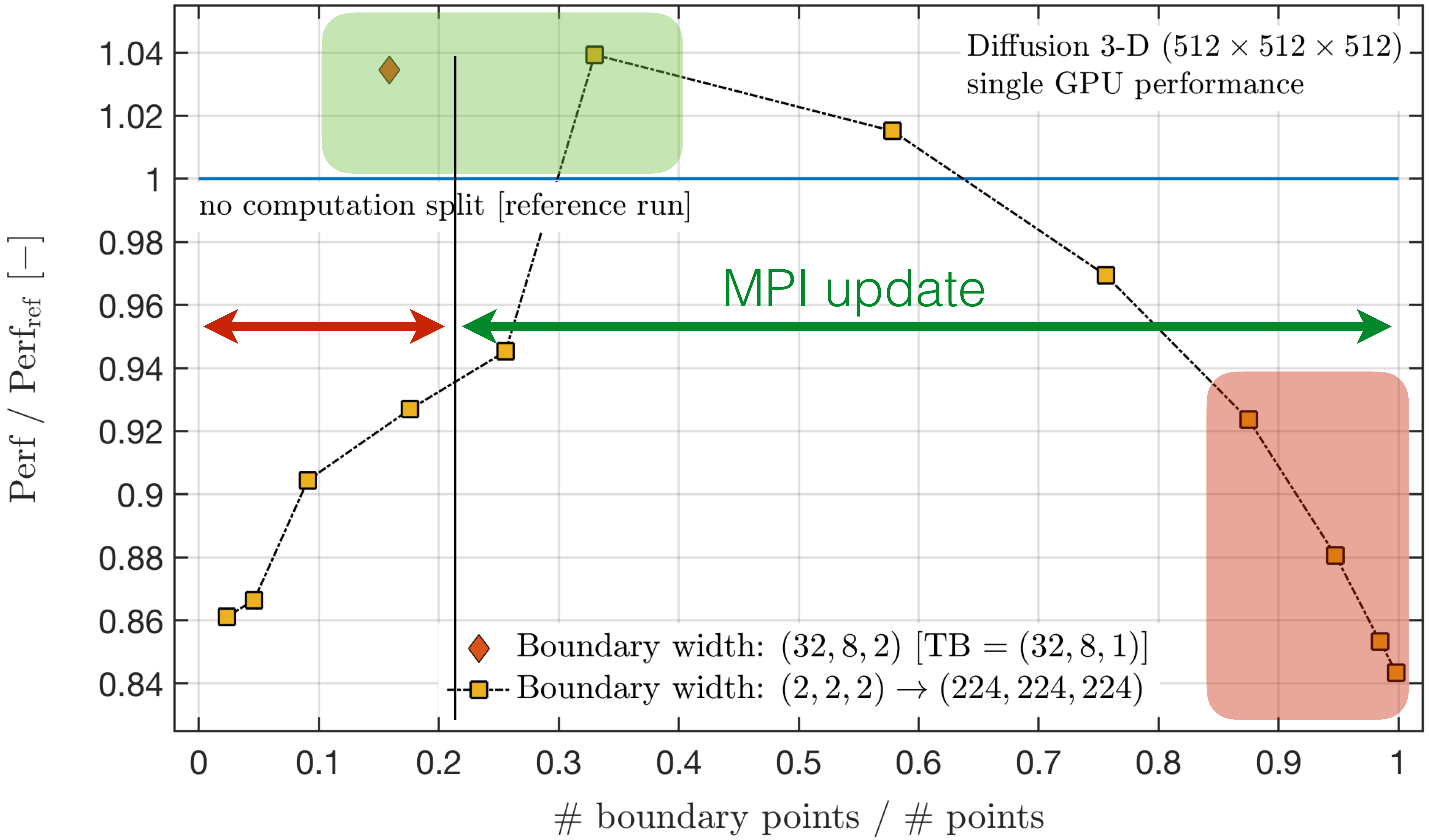
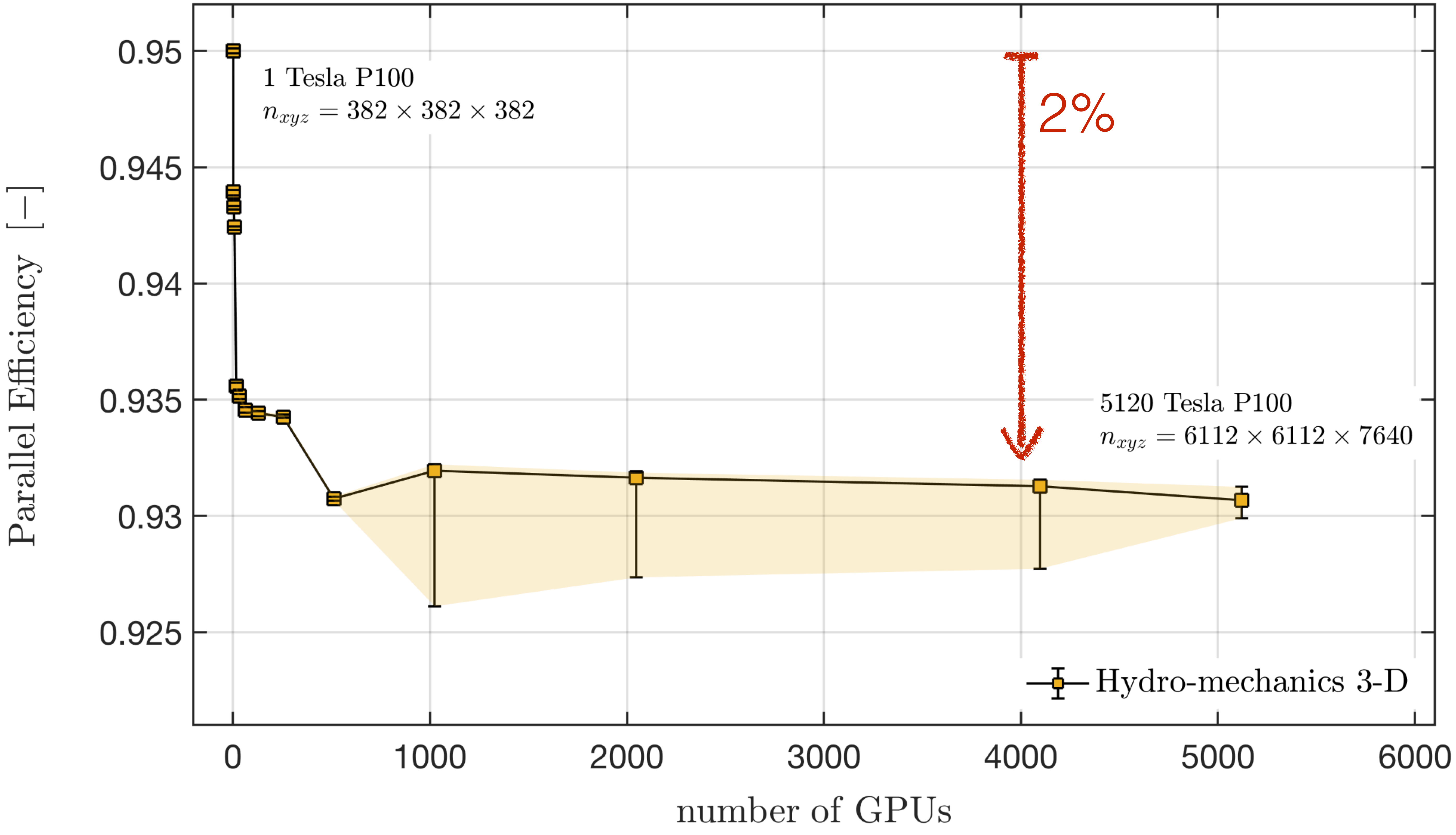


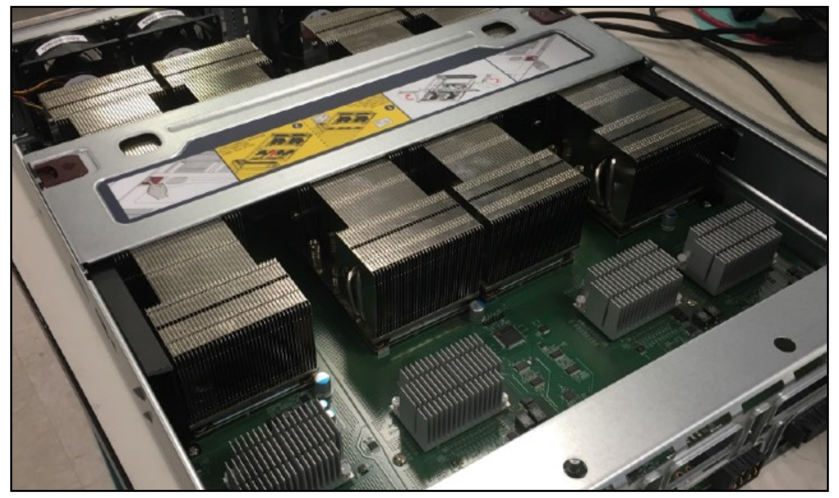
Parallel efficiency

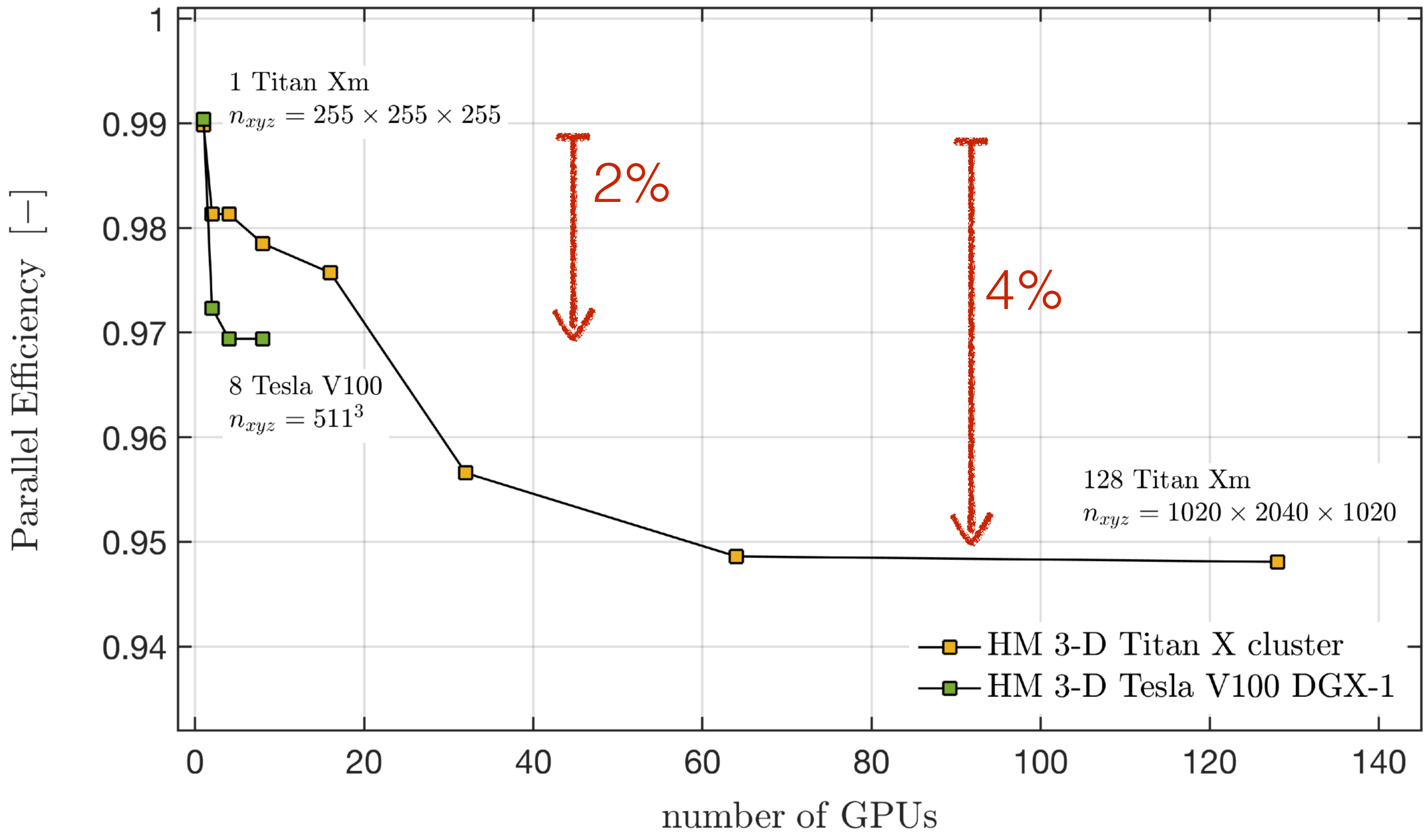
- 2% drop on 5120 Tesla P100 GPUs on Cray XC50 "Piz Daint" @ CSCS



Parallel efficiency

- In-house: 4% drop on 128 Titan Xm GPUs on in-house supercomputer “Octopus” @ Unil
  2% drop on 8 Tesla V100 Nvlink GPUs (DGX-1) “Volta” @ Unil





2/ Parallel efficiency

Summary

- Only 2% drop of parallel efficiency on 5120 GPUs compared to single GPU execution
- CudaStream: simple approach to access GPU memory while computations are ongoing
- Boundary width > 2, can avoid loss of performance when splitting computations
- Avoid blocking the computing and prioritise boundary update workflow
- Only minimal changes to original code - even for real-world applications !

Summary

We tackled hardware limit with our multi-GPU 3-D solver

- 1/ Using simple physics-based fast local iterative scheme
  > Pseudo-time brings physics back

- 2/ Implementing domain decomposition and asynchronous execution to hide MPI
  > Scale on the world's fastest supercomputers

Summary

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- 1/ Using simple physics-based fast local iterative scheme
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  > Scale on the world's fastest supercomputers

A general approach that is not restricted to our particular geo-physics application

Outlook

This approach can be applied to a wide range of computational physics problems

- Get the most out of a tight interplay

- Improve the effective memory throughput of our solver | MTP_{eff} @ ~25% of memcpy
- What's next: Testing PT iterations for for Finite-Elements
- What's next: Application to various coupled physical processes in Earth sciences

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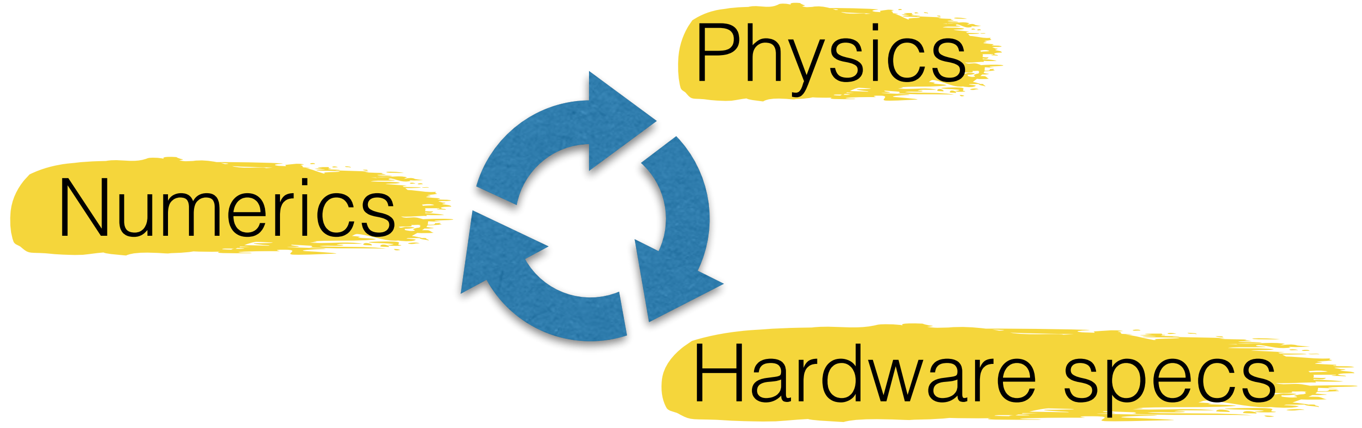

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Thank you

CSCS
Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

COLFAX
Customized Solutions

Unil
UNIL | Université de Lausanne
Swiss Geocomputing Centre

FNSNF
FONDS NATIONAL SUISSE
SCHWEIZERISCHER NATIONALFONDS
FONDO NAZIONALE SVIZZERO
SWISS NATIONAL SCIENCE FOUNDATION

SIGMA

Stanford University

Thank you

wp.unil.ch/geocomputing/

lraess@stanford.edu

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Løseth, H., Wensaas, L., Arntsen, B., Hanken, N.-M., Basire, C., & Graue, K. (2011). 1000 m long gas blow-out pipes. *Marine and Petroleum Geology*, *28*(5), 1047–1060.

Plaza-Faverola, A., Bünz, S., & Mienert, J. (2011). Repeated fluid expulsion through sub-seabed chimneys offshore Norway in response to glacial cycles. *Earth and Planetary Science Letters*, *305*(3–4), 297–308.

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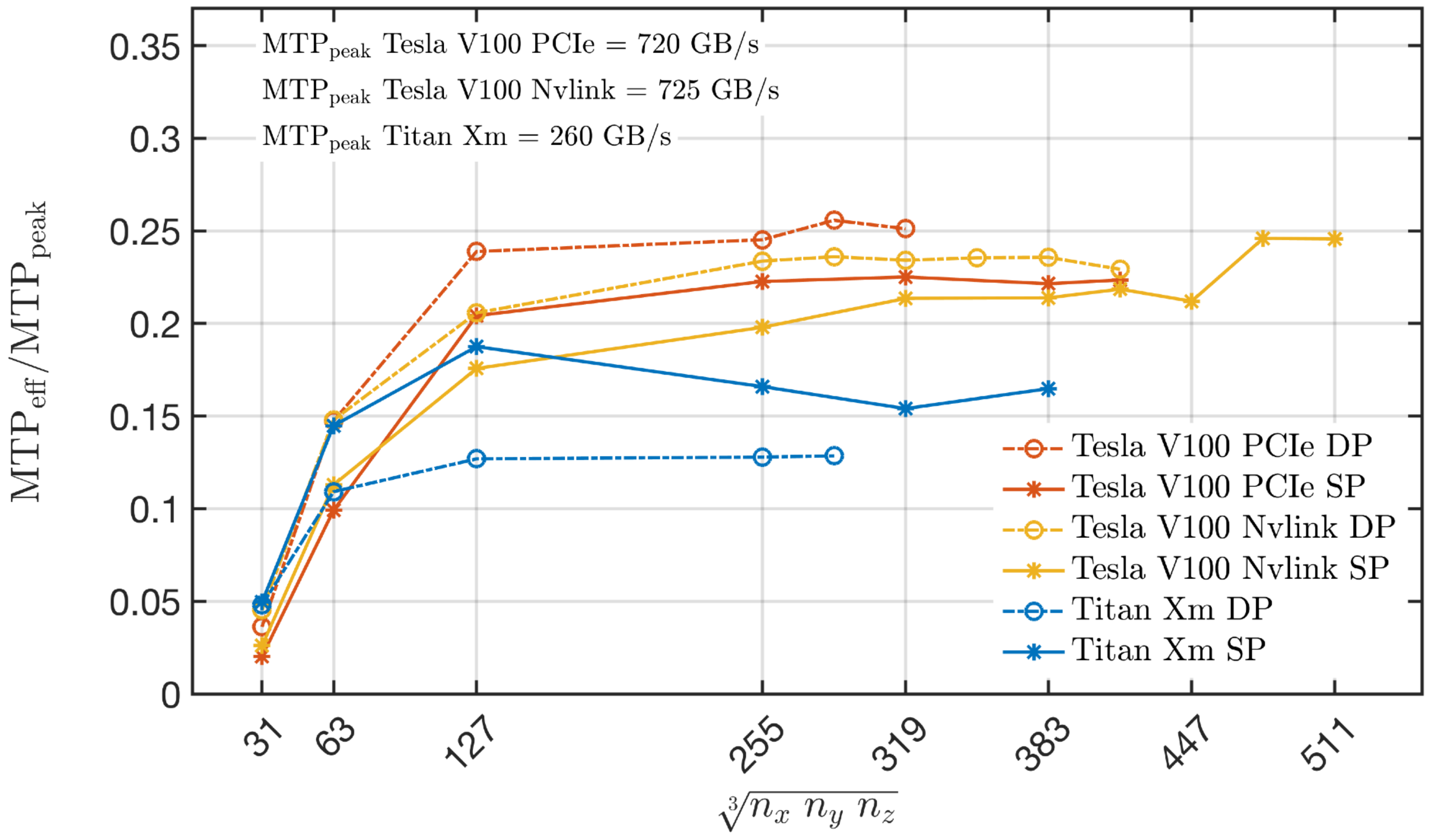
Effective memory throughput

Effective and absolute metric to measure optimality of data access: $MTP_{effective}$

- Minimal # of memory access / iteration: 15 read + write (30 accesses)
- MTP_{peak} = memcpy only
- $MTP_{eff} < MTP_{peak}$: no neighbours read or access (derivatives) counted but they occur - (a stencil code).



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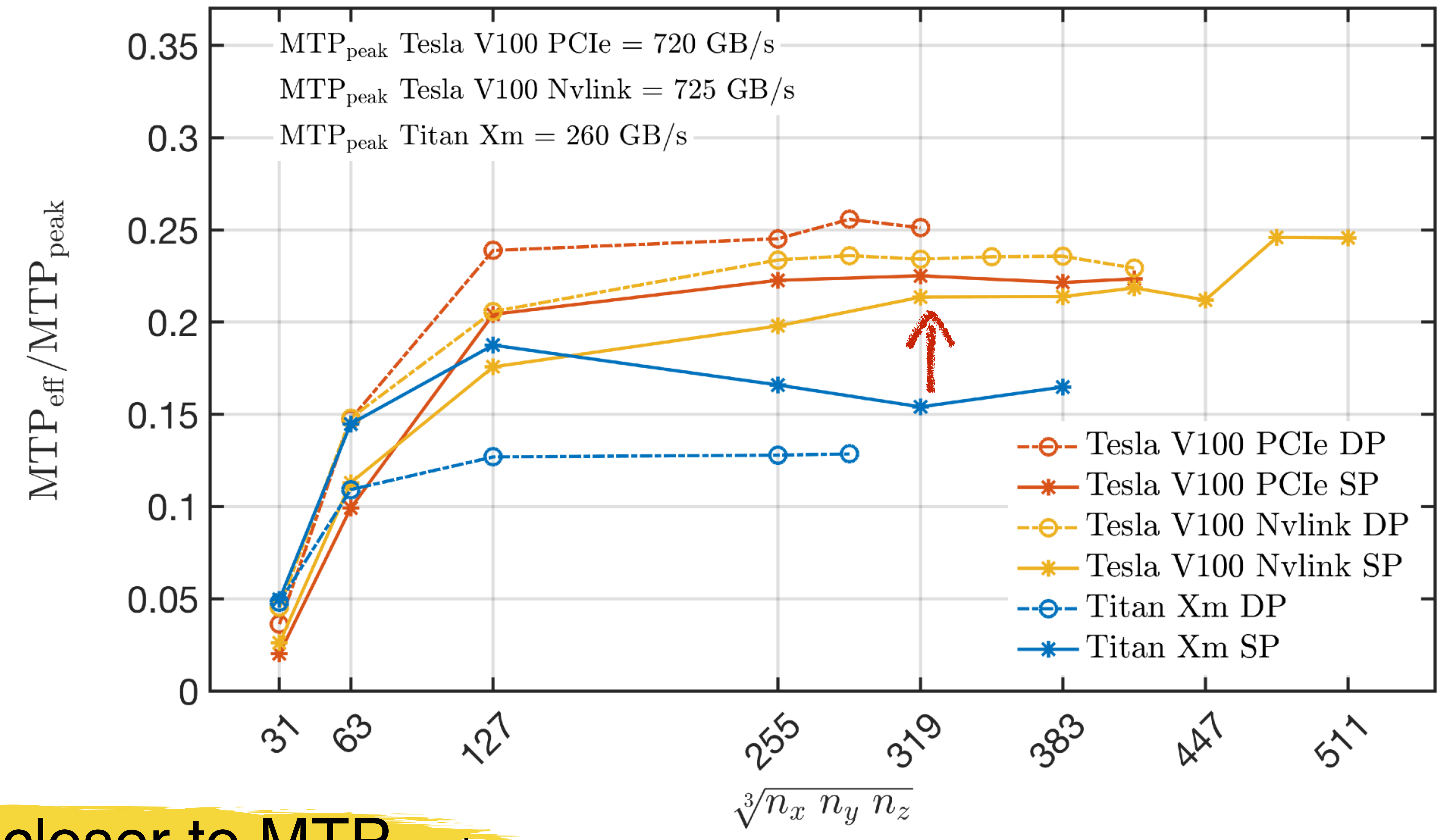
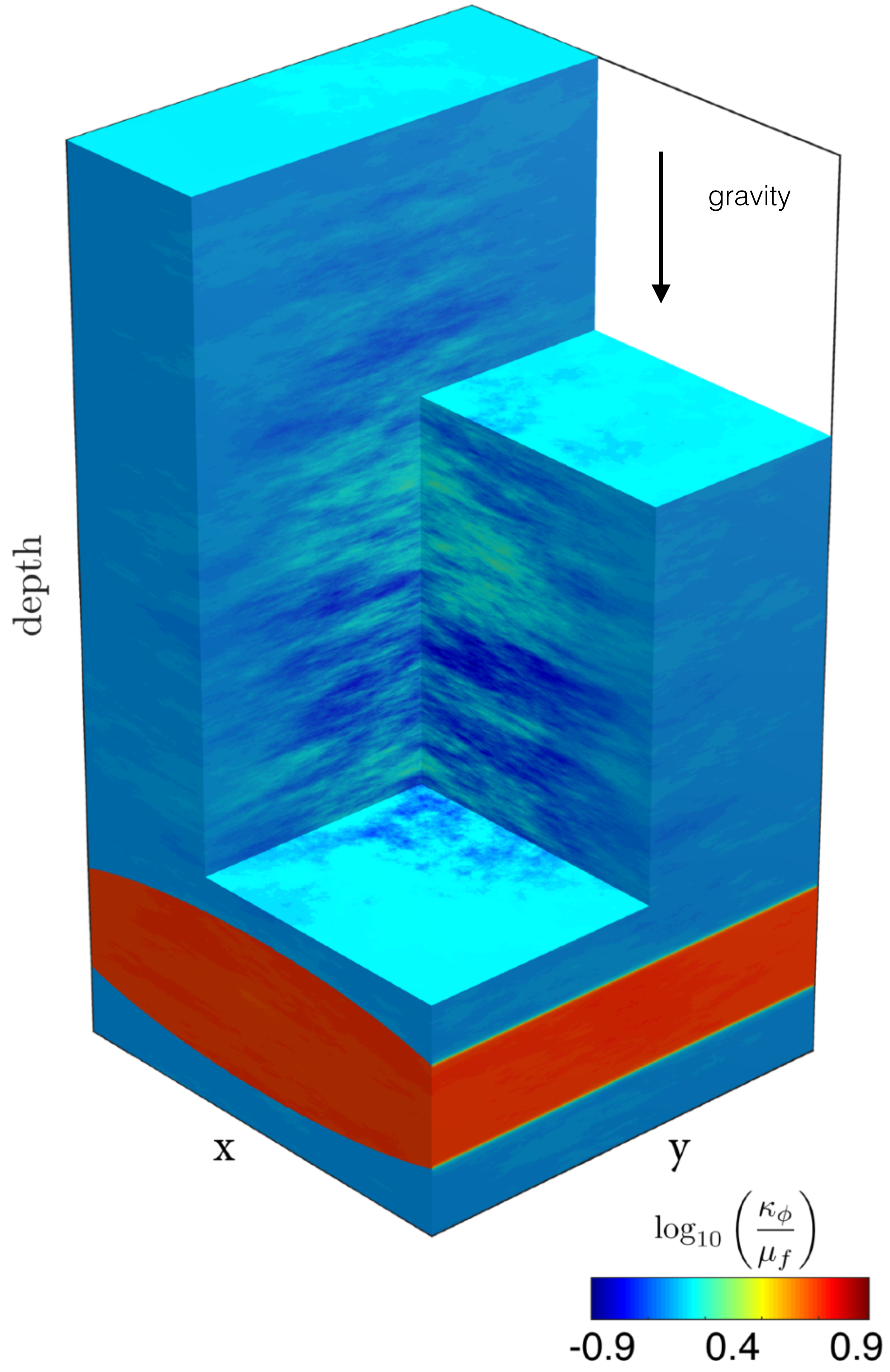


Future goes closer to MTP_{peak}

3-D fully coupled hydro-mechanics

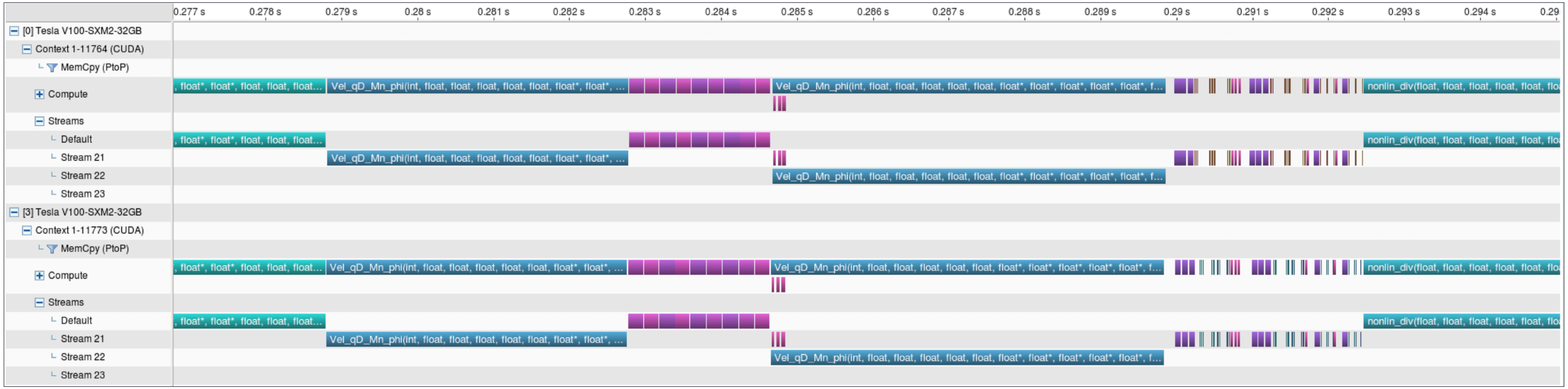
Spontaneous formation: 3-D numerical simulation

- Sediment deformation coupled to fluid motion
- Buoyancy driven flow: $\rho^{\mathrm{s}} = 2\rho^{\mathrm{f}}$
- Nonlinear mechanics (tensor + vector fields)
- Nonlinear fluid flow (vector field)
- Very high resolution:
  - space: 1000 x 1000 x 2000 grid points in 3-D
  - time: 20’000 time steps



Hiding communication

- Wrong implementation of CudaStream with blocking call to cudaDeviceSynchronize();



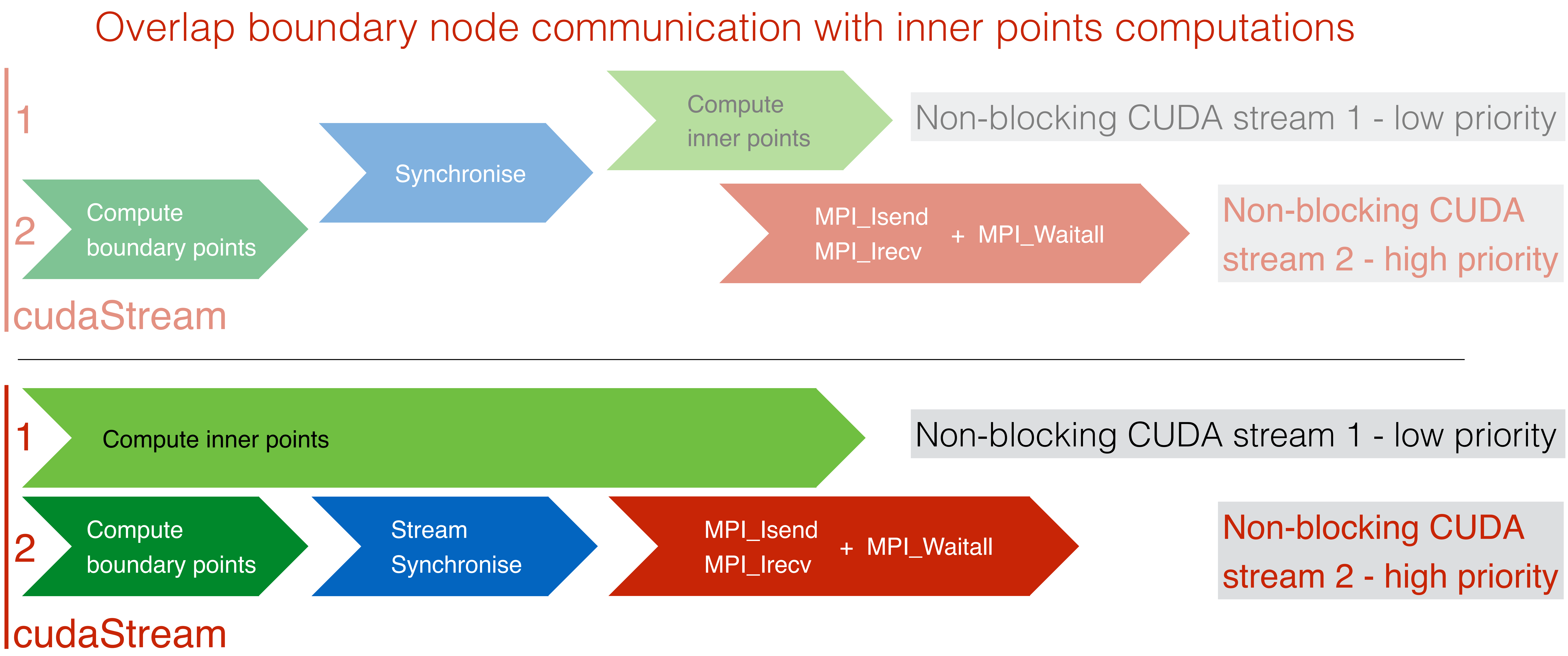
cudaStream implementation

CudaStream: simple approach to access memory on GPU while computations are ongoing:

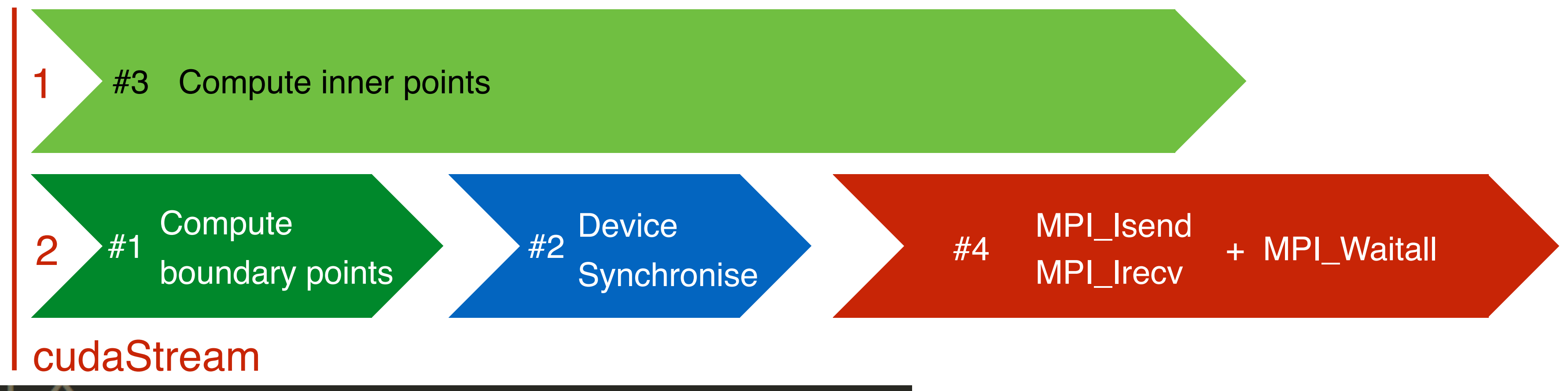
- Non blocking data accesses on the GPU as they happen on different non-blocking streams > flag for stream creation: `cudaStreamNonBlocking`.
- Syncing [Update boundaries] kernel does not interfere with [Compute inner points] kernel as it is done for stream 2 only: `cudaStreamSynchronize()`.
- Higher priority of stream 2 vs stream 1: `cudaStreamCreateWithPriority()`.
- Boundary width > 2 ensures optimal performance.

Hiding communication 2

- Alternative approach



Minimal changes to the code 2

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#define BOUNDARY_WIDTH_Y 32
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__global__ void compute(int istep){
    int ix = blockIdx.x*blockDim.x + threadIdx.x; // thread ID, dimension x
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    // Return if no work to do.
    if (   istep==0 &&     ix>=BOUNDARY_WIDTH_X && ix<=nx-1-BOUNDARY_WIDTH_X &&
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    //(...) (rest of the kernel as before)
}

main(){
    //(...)
    for (int istep=0; istep<2; istep++){
        compute<<<grid,block,0,streams[istep]>>>(istep);     // step 1 (istep==0) and step 3 (istep==1)
        if (istep==0) cudaStreamSynchronize(stream[0]);      // step 2
    }
    update_boundaries();                                      // step 4
    //(...)
}
```

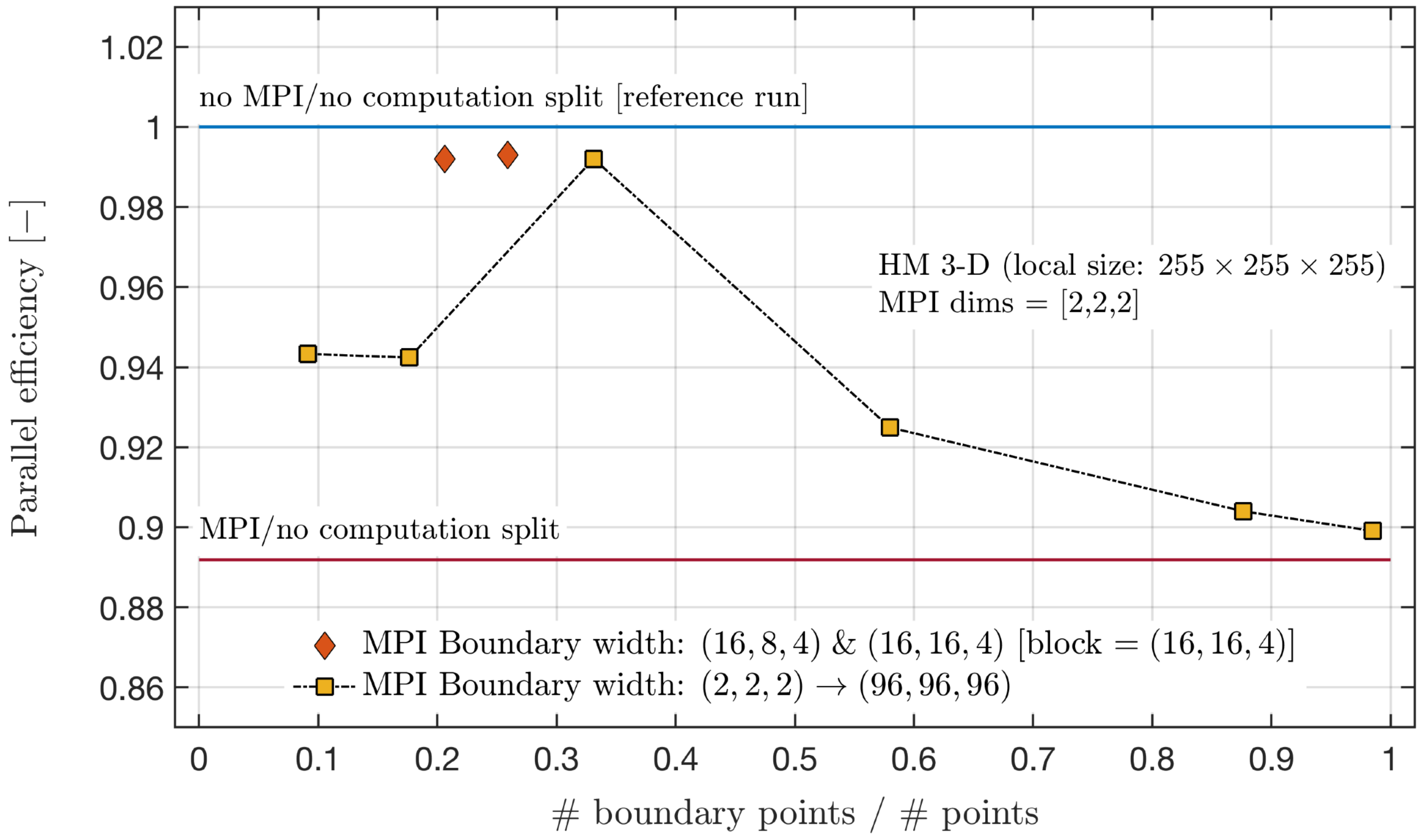
Hiding communication 2

Alternative approach for hiding MPI communication

- Synchronise only stream 2 (`cudaStreamSynchronize` instead of `cudaDeviceSynchronize`): only 1 modification to switch between two approaches !
- [compute inner points] begins simultaneous with [compute boundary points] kernels
- (+) No performance lost: boundary points & inner points are computed at the same time
- (-) Strongly rely on the stream priority feature to work very well
- (-) The less the priority is respected, the more the MPI data transfer begin will be delayed
- (-) Difficult to predict the time available for the MPI update

Avoid loss of performance

- Impact on the parallel efficiency | similar trend



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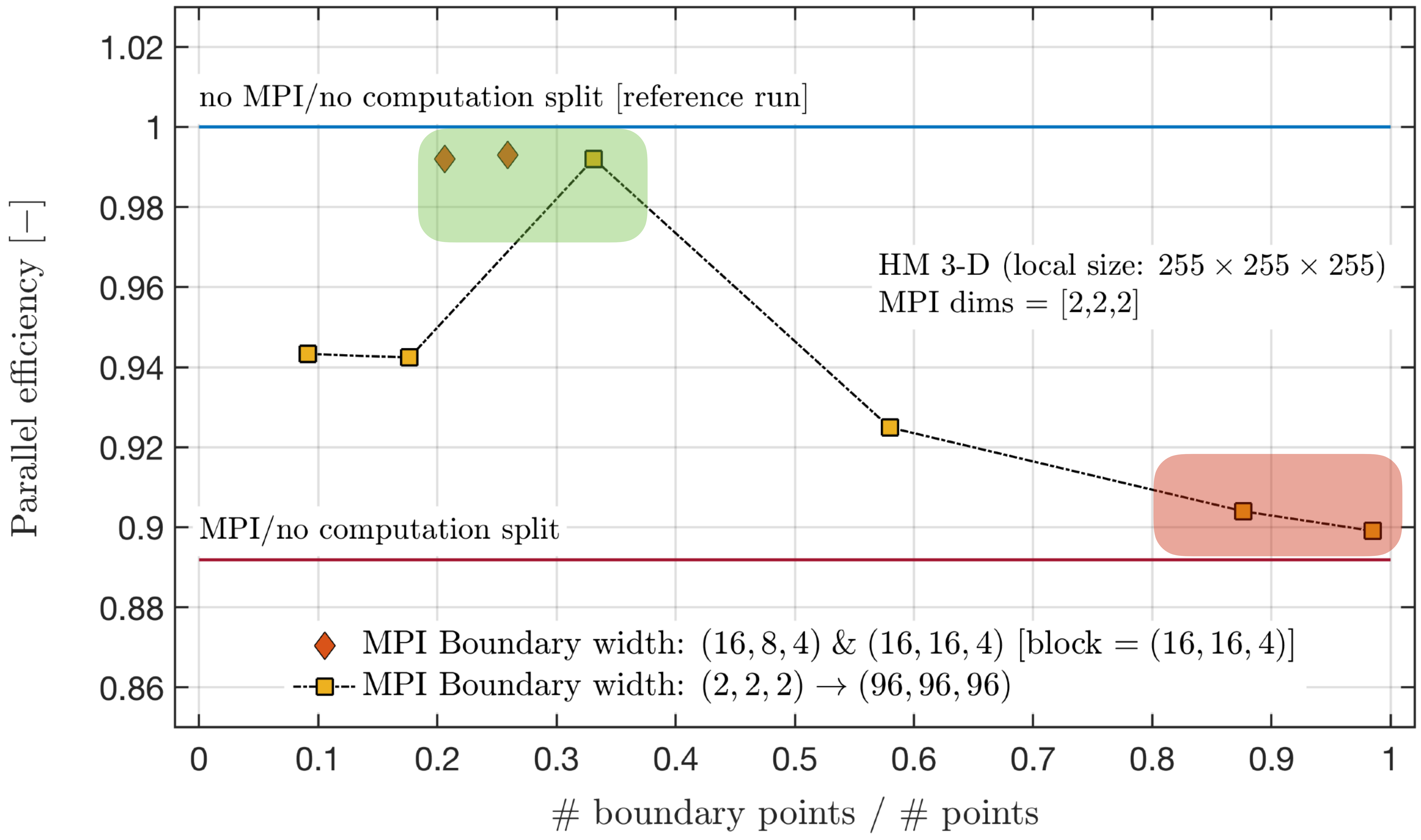

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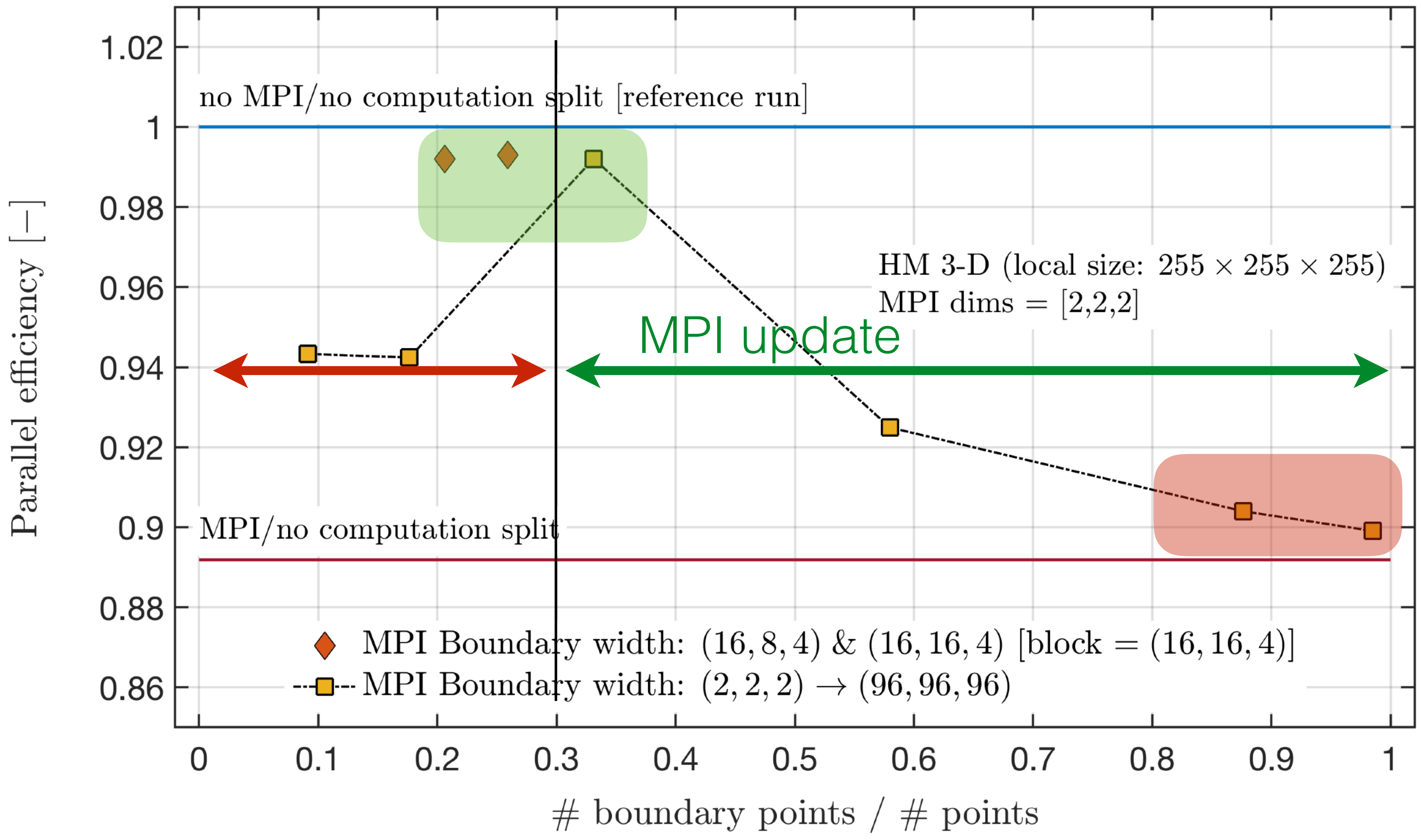

Optimality of data access

Optimality of data access

- PDE solvers are memory bound: computations $ | memory accesses $$$$
- Choose an appropriate solution strategy (solver):
  - Low memory footprint algorithm
  - Simple and regular data access pattern
- Computations are for free: recompute fields instead of storing them

/!\ High $MTP_{eff} \neq$ fast convergence (low # of iterations)

Performance limiters

- 15 fields to update R+W
- Bytes ≠ numbers (here float = 4 bytes)
- Current = main memory + cache
- Upper bound = minimal n_{IO}
- ratio = flops/bytes

0.1 < 1.8 << machine balances (17 or 24)

We are memory bound

3-D hydro-mechanics

Operation	Count	# flops	# bytes (float)	ratio
R+W	15	0	120	
$\frac{\partial}{\partial x}$	31	62	372	
Total (current)		62	524	0.1

GPU	# flops	# bytes (float)	ratio
Tesla V100	15.7×10^{12}	0.9×10^{12}	17
Titan Xm	12.1×10^{12}	0.5×10^{12}	24

Effective memory throughput

- Use an effective and absolute metric to measure optimality of data access: $\mathrm{MTP_{eff}}$
- Minimal # of memory transfers / iteration: $n_{\mathrm{RW}} = 30$ (R+W every 15 variable once)
- Tells us how far we are from ideal: compare to $\mathrm{MTP_{peak}}$ (memcopy only - no flops)

$$\boxed{\mathrm{MTP_{eff}} = \frac{n_{\mathrm{RW}}\, n_i^{\mathrm{tot}}\, n_{\mathrm{precis}}}{2^{30}\, t_{\mathrm{elapsed}}} \quad [\mathrm{GB/s}]}$$

$$\begin{aligned} n_{\mathrm{RW}} &= 2 \times (\text{read and write}) + \text{read only fields} \\ n_i^{\mathrm{tot}} &= n_x \times n_y \times n_z \times n_{\mathrm{t}} \\ n_{\mathrm{precis}} &= \text{word size [bytes]} \\ t_{\mathrm{elapsed}} &= \text{elapsed time [sec]} \end{aligned}$$

$\mathrm{MTP_{eff}}$ = lower bound of required memory transfers / time per iteration

$\neq$

$\mathrm{MTP_{profiler}}$ = performed memory transfers / time per iteration